

Generalised additive and index models with shape constraints

Yining Chen and Richard J. Samworth
Statistical Laboratory
University of Cambridge
{y.chen, r.samworth}@statslab.cam.ac.uk

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Abstract

We study generalised additive models, with shape restrictions (e.g. monotonicity, convexity, concavity) imposed on each component of the additive prediction function. We show that this framework facilitates a nonparametric estimator of each additive component, obtained by maximising the likelihood. The procedure is free of tuning parameters and under mild conditions is proved to be uniformly consistent on compact intervals. More generally, our methodology can be applied to generalised additive index models. Here again, the procedure can be justified on theoretical grounds and, like the original algorithm, possesses highly competitive finite-sample performance. Practical utility is illustrated through the use of these methods in the analysis of two real datasets. Our algorithms are publicly available in the R package `scar`, short for shape-constrained additive regression.

Keywords: Generalised additive models, Index models, Nonparametric maximum likelihood estimation, Shape constraints.

1 Introduction

Generalised additive models (GAMs) (Hastie and Tibshirani, 1986, 1990; Wood, 2006) have become an extremely popular tool for modelling multivariate data. They are designed to enjoy the flexibility of nonparametric modelling while avoiding the curse of dimensionality (Stone, 1986). Mathematically, suppose that we observe pairs $(\mathbf{X}_1, Y_1), \dots, (\mathbf{X}_n, Y_n)$, where $\mathbf{X}_i = (X_{i1}, \dots, X_{id})^T \in \mathbb{R}^d$ is the predictor and $Y_i \in \mathbb{R}$ is the response, for $i = 1, \dots, n$. A generalised additive model relates the

predictor and the mean response $\mu_i = \mathbb{E}(Y_i)$ through

$$g(\mu_i) = f(\mathbf{X}_i) = \sum_{j=1}^d f_j(X_{ij}) + c,$$

where g is a specified link function, and where the response Y_i follows an exponential family distribution. Here $c \in \mathbb{R}$ is the intercept term and for every $j = 1, \dots, d$, the additive component function $f_j : \mathbb{R} \rightarrow \mathbb{R}$ is assumed to satisfy the identifiability constraint $f_j(0) = 0$. Our aim is to estimate the additive components f_1, \dots, f_d together with the intercept c based on the given observations. Standard estimators are based on penalised spline-based methods (e.g. Wood, 2004, 2008), and involve tuning parameters whose selection is not always straightforward, especially if different additive components have different levels of smoothness, or if individual components have non-homogeneous smoothness.

In this paper, we propose a new approach, motivated by the fact that the additive components of f often follow certain common shape constraints such as monotonicity or convexity. The full list of constraints we consider is given in Table 1, with each assigned a numerical label to aid our exposition. By assuming that each of f_1, \dots, f_d satisfies one of these nine shape restrictions, we show in Section 2 that it is possible to derive a nonparametric maximum likelihood estimator, which requires no choice of tuning parameters and which can be computed using fast convex optimisation techniques. In Theorem 2, we prove that under mild regularity conditions, it is uniformly consistent on compact intervals.

shape constraint	label	shape constraint	label	shape constraint	label
linear	1	monotone increasing	2	monotone decreasing	3
convex	4	convex increasing	5	convex decreasing	6
concave	7	concave increasing	8	concave decreasing	9

Table 1: Different shape constraints and their corresponding labels

More generally, as we describe in Section 3, our approach can be applied to generalised additive index models (GAIMs), in which the predictor and the response are related through

$$g(\mu_i) = f^I(\mathbf{X}_i) = f_1(\boldsymbol{\alpha}_1^T \mathbf{X}_i) + \dots + f_m(\boldsymbol{\alpha}_m^T \mathbf{X}_i) + c, \quad (1)$$

where the value of $m \in \mathbb{N}$ is assumed known, where g is a known link function, and where the response Y_i again follows an exponential family distribution. Here, $\boldsymbol{\alpha}_1, \dots, \boldsymbol{\alpha}_m \in \mathbb{R}^d$ are called the *projection indices*, $f_1, \dots, f_m : \mathbb{R} \rightarrow \mathbb{R}$ are called the *ridge functions* (or sometimes, *additive*

components) of f^I , and $c \in \mathbb{R}$ is the intercept. Such index models have also been widely applied, especially in the area of econometrics (Li and Racine, 2007). When g is the identity function, the model is also known as projection pursuit regression (Friedman and Stuetzle, 1981); when $m = 1$, the model reduces to the single index model (Ichimura, 1993). By imposing shape restrictions on each of f_1, \dots, f_m , we extend our methodology and theory to this setting, allowing us to estimate simultaneously the projection indices, the ridge functions and the intercept.

The challenge of computing our estimators is taken up in Section 4, where our algorithms are described in detail. In Section 5, we summarise the results of a thorough simulation study designed to compare the finite-sample properties of **scar** with several alternative procedures. We conclude in Section 6 with two applications of our methodology to real datasets concerning doctoral publications in biochemistry and the decathlon. The proofs of our main results can be found in the Appendix; various auxiliary results are given in the online supplementary material.

This paper contributes to the larger literature of regression in the presence of shape constraints. In the univariate case, and with the identity link function, the properties of shape-constrained least squares procedures are well-understood, especially for the problem of isotonic regression. See, for instance, Brunk (1958), Brunk (1970) and Barlow *et al.* (1972). For the problem of univariate convex regression, see Hanson and Pledger (1976), Groeneboom, Jongbloed and Wellner (2001), Groeneboom, Jongbloed and Wellner (2008) and Guntuboyina and Sen (2013). These references cover consistency, local and global rates of convergence, and computational aspects of the estimator. Mammen and Yu (2007) studied additive isotonic regression with the identity link function. During the preparation of this manuscript, we became aware of the work of Meyer (2013a), who developed similar methodology (but not theory) to ours in the Gaussian, non-index setting. The problem of GAMs with shape restrictions was also recently studied by Pya and Wood (2014), who proposed a penalised spline method that is compared with ours in Section 5. Finally, we mention that recent work by Kim and Samworth (2014) has shown that shape-restricted inference without further assumptions can lead to slow rates of convergence in higher dimensions. The additive or index structure therefore becomes particularly attractive in conjunction with shape constraints as an attempt to evade the curse of dimensionality.

2 Generalised additive models with shape constraints

2.1 Maximum likelihood estimation

Recall that the density function of a natural exponential family (EF) distribution with respect to a reference measure (either Lebesgue measure on \mathbb{R} or counting measure on \mathbb{Z}) can be written in the form

$$f_Y(y; \mu, \phi) = h(y, \phi) \exp \left\{ \frac{yg(\mu) - B(g(\mu))}{\phi} \right\},$$

where $\mu \in \mathcal{M} \subseteq \mathbb{R}$ and $\phi \in \Phi \subseteq (0, \infty)$ are the mean and dispersion parameters respectively. To simplify our discussion, we restrict our attention to the most commonly-used natural EF distributions, namely, the Gaussian, Gamma, Poisson and Binomial families, and take g to be the canonical link function. Expressions for g and the (strictly convex) log-partition function B for the different exponential families can be found in Table 2. The corresponding distributions are denoted by $\text{EF}_{g,B}(\mu, \phi)$, and we write $\text{dom}(B) = \{\eta \in \mathbb{R} : B(\eta) < \infty\}$ for the domain of B . As a convention, for the Binomial family, the response is scaled to take values in $\{0, 1/T, 2/T, \dots, 1\}$ for some known $T \in \mathbb{N}$.

exponential family	$g(\mu)$	$B(\eta)$	$\text{dom}(B)$	\mathcal{M}	Φ
Gaussian	μ	$\eta^2/2$	\mathbb{R}	\mathbb{R}	$(0, \infty)$
Gamma	$-\mu^{-1}$	$-\log(-\eta)$	$(-\infty, 0)$	$(0, \infty)$	$(0, \infty)$
Poisson	$\log \mu$	e^η	\mathbb{R}	$(0, \infty)$	$\{1\}$
Binomial	$\log \frac{\mu}{1-\mu}$	$\log(1 + e^\eta)$	\mathbb{R}	$(0, 1)$	$\{1/T\}$

Table 2: Exponential family distributions, their corresponding canonical link functions, log-partition functions and mean and dispersion parameter spaces.

If $(\mathbf{X}_1, Y_1), \dots, (\mathbf{X}_n, Y_n)$ are independent and identically distributed pairs taking values in $\mathbb{R}^d \times \mathbb{R}$, with $Y_i | \mathbf{X}_i \sim \text{EF}_{g,B}(g^{-1}(f(\mathbf{X}_i)), \phi)$ for some *prediction function* $f : \mathbb{R}^d \rightarrow \text{dom}(B)$, then the (conditional) log-likelihood of f can be written as

$$\frac{1}{\phi} \sum_{i=1}^n \{Y_i f(\mathbf{X}_i) - B(f(\mathbf{X}_i))\} + \sum_{i=1}^n \log h(Y_i, \phi).$$

Since we are only interested in estimating f , it suffices to consider the *scaled partial log-likelihood*

$$\bar{\ell}_{n,d}(f) \equiv \bar{\ell}_{n,d}(f; (\mathbf{X}_1, Y_1), \dots, (\mathbf{X}_n, Y_n)) := \frac{1}{n} \sum_{i=1}^n \{Y_i f(\mathbf{X}_i) - B(f(\mathbf{X}_i))\} \equiv \frac{1}{n} \sum_{i=1}^n \ell_{i,d}(f),$$

say. In the rest of this section, and in the proof of Proposition 1 and Theorem 2 in the appendix, we suppress the dependence of $\bar{\ell}_{n,d}(\cdot)$ and $\ell_{i,d}(\cdot)$ on d in our notation.

Let $\bar{\mathbb{R}} = \mathbb{R} \cup \{-\infty, \infty\}$ denote the extended real line. In order to guarantee the existence of our estimator, it turns out to be convenient to extend the definition of each ℓ_i (and therefore $\bar{\ell}_n$) to all $f : \mathbb{R}^d \rightarrow \bar{\mathbb{R}}$, which we do as follows:

1. For the Gamma family, if $f(\mathbf{X}_i) \geq 0$, then we take $\ell_i(f) = -\infty$. This is because the log-partition function of the Gamma family has domain $(-\infty, 0)$, so f must be negative at \mathbf{X}_i in order for $\ell_i(f)$ to be well-defined.
2. If $f(\mathbf{X}_i) = -\infty$, then we set $\ell_i(f) = \lim_{a \rightarrow -\infty} Y_i a - B(a)$. Similarly, if $f(\mathbf{X}_i) = \infty$ (in the Gaussian, Poisson or Binomial setting), then we define $\ell_i(f) = \lim_{a \rightarrow \infty} Y_i a - B(a)$. Note that both limits always exist in $\bar{\mathbb{R}}$.

For any $\mathbf{L}_d = (l_1, \dots, l_d)^T \in \{1, 2, \dots, 9\}^d$, let $\mathcal{F}^{\mathbf{L}_d}$ denote the set of functions $f : \mathbb{R}^d \rightarrow \mathbb{R}$ of the form

$$f(\mathbf{x}) = \sum_{j=1}^d f_j(x_j) + c$$

for $\mathbf{x} = (x_1, \dots, x_d)^T \in \mathbb{R}^d$, where for every $j = 1, \dots, d$, $f_j : \mathbb{R} \rightarrow \mathbb{R}$ is a function obeying the shape restriction indicated by label l_j and satisfying $f_j(0) = 0$, and where $c \in \mathbb{R}$. Whenever f has such a representation, we write $f \stackrel{\mathcal{F}^{\mathbf{L}_d}}{\sim} (f_1, \dots, f_d, c)$, and call \mathbf{L}_d the *shape vector*. The pointwise closure of $\mathcal{F}^{\mathbf{L}_d}$ is defined as

$$\text{cl}(\mathcal{F}^{\mathbf{L}_d}) = \left\{ f : \mathbb{R}^d \rightarrow \bar{\mathbb{R}} \mid \exists f^1, f^2, \dots \in \mathcal{F}^{\mathbf{L}_d} \text{ s.t. } \lim_{k \rightarrow \infty} f^k(\mathbf{x}) = f(\mathbf{x}) \text{ for every } \mathbf{x} \in \mathbb{R}^d \right\}.$$

For a specified shape vector \mathbf{L}_d , we define the shape-constrained maximum likelihood estimator (SCMLE) as

$$\hat{f}_n \in \underset{f \in \text{cl}(\mathcal{F}^{\mathbf{L}_d})}{\operatorname{argmax}} \bar{\ell}_n(f).$$

Like other shape restricted regression estimators, \hat{f}_n is not unique in general. However, as can be seen from the following proposition, the value of \hat{f}_n is uniquely determined at $\mathbf{X}_1, \dots, \mathbf{X}_n$.

Proposition 1. *The set $\hat{S}_n^{\mathbf{L}_d} = \operatorname{argmax}_{f \in \text{cl}(\mathcal{F}^{\mathbf{L}_d})} \bar{\ell}_n(f)$ is non-empty. Moreover, all elements of $\hat{S}_n^{\mathbf{L}_d}$ agree at $\mathbf{X}_1, \dots, \mathbf{X}_n$.*

Remarks:

1. As can be seen from the proof of Proposition 1, if the EF distribution is Gaussian or Gamma, then $\hat{S}_n^{\mathbf{L}_d} \cap \mathcal{F}^{\mathbf{L}_d} \neq \emptyset$.
2. Under the Poisson setting, if $Y_i = 0$, then it might happen that $\hat{f}_n(\mathbf{X}_i) = -\infty$. Likewise, for the Binomial GAM, if $Y_i = 0$ or 1 , then it is possible to have $\hat{f}_n(\mathbf{X}_i) = -\infty$ or ∞ , respectively. This is why we maximise over the closure of $\mathcal{F}^{\mathbf{L}_d}$ in our definition of SCMLE.

2.2 Consistency of the SCMLE

In this subsection, we show the consistency of \hat{f}_n in a random design setting. We will impose the following assumptions:

- (A.1) $(\mathbf{X}, Y), (\mathbf{X}_1, Y_1), (\mathbf{X}_2, Y_2), \dots$ is a sequence of independent and identically distributed pairs taking values in $\mathbb{R}^d \times \mathbb{R}$.
- (A.2) The random vector \mathbf{X} has a Lebesgue density with support \mathbb{R}^d .
- (A.3) Fix $\mathbf{L}_d \in \{1, 2, \dots, 9\}^d$. Suppose that $Y|\mathbf{X} \sim \text{EF}_{g,B}(g^{-1}(f_0(\mathbf{X})), \phi_0)$, where $f_0 \in \mathcal{F}^{\mathbf{L}_d}$ and $\phi_0 \in (0, \infty)$ denote the true prediction function and dispersion parameter respectively.
- (A.4) f_0 is continuous on \mathbb{R}^d .

We are now in the position to state our main consistency result:

Theorem 2. *Assume (A.1) – (A.4). Then, for every $a_0 \geq 0$,*

$$\sup_{\hat{f}_n \in \hat{S}_n^{\mathbf{L}_d}} \sup_{\mathbf{x} \in [-a_0, a_0]^d} |\hat{f}_n(\mathbf{x}) - f_0(\mathbf{x})| \xrightarrow{a.s.} 0$$

as $n \rightarrow \infty$.

Remarks:

1. When the EF distribution is Gaussian, SCMLE coincides with the shape-constrained least squares estimator (SCLSE). Using essentially the same argument, one can prove the the same consistency result for the SCLSE under a slightly different setting where $Y_i = f_0(\mathbf{X}_i) + \epsilon_i$ for $i = 1, \dots, n$, and where $\epsilon_1, \dots, \epsilon_n$ are independent and identically distributed with zero mean and finite variance, but are not necessarily Gaussian.
2. Assumption (A.2) can be weakened at the expense of lengthening the proof still further. For instance, one can assume only that the support $\text{supp}(\mathbf{X})$ of the covariates to be a convex subset of \mathbb{R}^d with positive Lebesgue measure. In that case, it can be concluded that \hat{f}_n converges uniformly to f_0 almost surely on any compact subset contained in the interior of $\text{supp}(\mathbf{X})$. In fact, with some minor modifications, our proof can also be generalised to situations where some components of \mathbf{X} are discrete.
3. Even without Assumption (A.4), consistency under a weaker norm can be established, namely

$$\sup_{\hat{f}_n \in \hat{S}_n^{\mathbf{L}_d}} \int_{[-a_0, a_0]^d} |\hat{f}_n(\mathbf{x}) - f_0(\mathbf{x})| d\mathbf{x} \xrightarrow{a.s.} 0, \quad \text{as } n \rightarrow \infty.$$

4. Instead of assuming a single dispersion parameter ϕ_0 as done here, one can take $\phi_{ni} = \phi_0/w_{ni}$ for $i = 1, \dots, n$, where w_{ni} are known, positive weights (this is frequently needed in practice in the Binomial setting). In that case, the new partial log-likelihood can be viewed as a

weighted version of the original one. Consistency of SCMLE can be established provided that $\liminf_{n \rightarrow \infty} \frac{\min_i w_{ni}}{\max_i w_{ni}} > 0$.

Under assumption **(A.3)**, we may write $f_0 \stackrel{\mathcal{F}^{\mathbf{L}_d}}{\sim} (f_{0,1}, \dots, f_{0,d}, c_0)$. From the proof of Theorem 2, we see that for any $a_0 > 0$, with probability one, for sufficiently large n , any $\hat{f}_n \in \hat{S}_n^{\mathbf{L}_d}$ can be written in the form $\hat{f}_n(\mathbf{x}) = \sum_{j=1}^d \hat{f}_{n,j}(x_j) + \hat{c}_n$ for $\mathbf{x} \in [-a_0, a_0]^d$, where $\hat{f}_{n,j}$ satisfies the shape constraint l_j and $\hat{f}_{n,j}(0) = 0$ for each $j = 1, \dots, d$. The following corollary establishes the important fact that each additive component (as well as the intercept term) is estimated consistently by SCMLE.

Corollary 3. *Assume **(A.1)** – **(A.4)**. Then, for any $a_0 \geq 0$,*

$$\sup_{\hat{f}_n \in \hat{S}_n^{\mathbf{L}_d}} \left\{ \sum_{j=1}^d \sup_{x_j \in [-a_0, a_0]} |\hat{f}_{n,j}(x_j) - f_{0,j}(x_j)| + |\hat{c}_n - c_0| \right\} \xrightarrow{a.s.} 0$$

as $n \rightarrow \infty$.

3 Generalised additive index models with shape constraints

3.1 The generalised additive index model and its identifiability

Recall that in the generalised additive index model, the response $Y_i \in \mathbb{R}$ and the predictor $\mathbf{X}_i = (X_{i1}, \dots, X_{id})^T \in \mathbb{R}^d$ are related through (1), where g is a known link function, and where conditional on \mathbf{X}_i , the response Y_i has a known EF distribution with mean parameter $g^{-1}(f(\mathbf{X}_i))$ and dispersion parameter ϕ .

Let $\mathbf{A} = (\boldsymbol{\alpha}_1, \dots, \boldsymbol{\alpha}_m)$ denote the $d \times m$ index matrix, where $m \leq d$, and let $f(\mathbf{z}) = \sum_{j=1}^m f_j(z_j) + c$ for $\mathbf{z} = (z_1, \dots, z_m)^T \in \mathbb{R}^m$, so the prediction function can be written as $f^I(\mathbf{x}) = f(\mathbf{A}^T \mathbf{x})$ for $\mathbf{x} = (x_1, \dots, x_d)^T \in \mathbb{R}^d$. As in Section 2, we impose shape constraints on the ridge functions by assuming that $f_j : \mathbb{R} \rightarrow \mathbb{R}$ satisfies the shape constraint with label $l_j \in \{1, 2, \dots, 9\}$, for $j = 1, \dots, m$.

To ensure the identifiability of the model, we only consider additive index functions f^I of the form (1) satisfying the following conditions, adapted from Yuan (2011):

- (B.1a)** $f_j(0) = 0$ for $j = 1, \dots, m$.
- (B.1b)** $\|\boldsymbol{\alpha}_j\|_1 = 1$ for $j = 1, \dots, m$, where $\|\cdot\|_1$ denotes the ℓ_1 norm.
- (B.1c)** The first non-zero entry of $\boldsymbol{\alpha}_j$ is positive for every j with $l_j \in \{1, 4, 7\}$.
- (B.1d)** There is at most one linear ridge function in f_1, \dots, f_m ; if f_k is linear, then $\boldsymbol{\alpha}_j^T \boldsymbol{\alpha}_k = 0$ for every $j \neq k$.
- (B.1e)** There is at most one quadratic ridge function in f_1, \dots, f_m .
- (B.1f)** \mathbf{A} has full column rank m .

3.2 GAIM estimation

Let $\mathbf{A}_0 = (\boldsymbol{\alpha}_{0,1}, \dots, \boldsymbol{\alpha}_{0,m})$ denote the true index matrix. For $\mathbf{x} = (x_1, \dots, x_d)^T \in \mathbb{R}^d$, let

$$f_0^I(\mathbf{x}) = f_{0,1}(\boldsymbol{\alpha}_{0,1}^T \mathbf{x}) + \dots + f_{0,m}(\boldsymbol{\alpha}_{0,m}^T \mathbf{x}) + c_0$$

be the true prediction function, and write $f_0(\mathbf{z}) = \sum_{j=1}^m f_{0,j}(z_j) + c_0$ for $\mathbf{z} = (z_1, \dots, z_m)^T \in \mathbb{R}^m$. Again we restrict our attention to the common EF distributions listed in Table 2 and take g to be the corresponding canonical link function. Let

$$\begin{aligned} \mathcal{A}_d^{\mathbf{L}_m} = \Big\{ \mathbf{A} = (\boldsymbol{\alpha}_1, \dots, \boldsymbol{\alpha}_m) \in \mathbb{R}^{d \times m} : \mathbf{A} \text{ satisfies assumptions (B.1b) -- (B.1c),} \\ \text{and if there exists } k \in \{1, \dots, m\} \text{ s.t. } l_k = 1, \text{ then } \boldsymbol{\alpha}_j^T \boldsymbol{\alpha}_k = 0 \text{ for every } j \neq k \Big\}. \end{aligned}$$

Given a shape vector \mathbf{L}_m , we consider the set of shape-constrained additive index functions given by

$$\mathcal{G}_d^{\mathbf{L}_m} = \left\{ f^I : \mathbb{R}^d \rightarrow \mathbb{R} \mid f^I(\mathbf{x}) = f(\mathbf{A}^T \mathbf{x}), \text{ with } f \in \mathcal{F}^{\mathbf{L}_m} \text{ and } \mathbf{A} \in \mathcal{A}_d^{\mathbf{L}_m} \right\},$$

A natural idea is to seek to maximise the scaled partial log-likelihood $\bar{\ell}_{n,d}$ over the pointwise closure of $\mathcal{G}_d^{\mathbf{L}_m}$. As part of this process, one would like to find a $d \times m$ matrix in $\mathcal{A}_d^{\mathbf{L}_m}$ that maximises the scaled partial *index log-likelihood*

$$\Lambda_n(\mathbf{A}) \equiv \Lambda_n\left(\mathbf{A}; (\mathbf{X}_1, Y_1), \dots, (\mathbf{X}_n, Y_n)\right) = \sup_{f \in \mathcal{F}^{\mathbf{L}_m}} \bar{\ell}_{n,m}\left(f; (\mathbf{A}^T \mathbf{X}_1, Y_1), \dots, (\mathbf{A}^T \mathbf{X}_n, Y_n)\right),$$

where the dependence of $\Lambda_n(\cdot)$ on \mathbf{L}_m is suppressed for notational convenience. We argue, however, that this strategy has two drawbacks:

1. **‘Saturated’ solution.** In certain cases, maximising $\Lambda_n(\mathbf{A})$ over $\mathcal{A}_d^{\mathbf{L}_m}$ can lead to a perfect fit of the model. We demonstrate this phenomenon via the following example.

Example 1. Consider the Gaussian family with the identity link function. We take $d = 2$. Assume that there are n observations $(\mathbf{X}_1, Y_1), \dots, (\mathbf{X}_n, Y_n)$ with $\mathbf{X}_i = (X_{i1}, X_{i2})^T$ and that $\mathbf{L}_2 = (2, 3)^T$. We assume here that $X_{11} < \dots < X_{n1}$. Note that it is possible to find an increasing function f_1 , an decreasing function f_2 (with $f_1(0) = f_2(0) = 0$) and a constant c such that $f_1(X_{i1}) + f_2(X_{i1}) + c = Y_i$ for every $i = 1, \dots, n$. Now pick ϵ such that

$$0 < \epsilon < \min \left\{ \frac{1}{2}, \frac{\min_{1 \leq i < n} (X_{i+1,1} - X_{i1})}{4(\max_{1 \leq i \leq n} |X_{i2}| + 1)} \right\},$$

and let $\mathbf{A} = (\boldsymbol{\alpha}_1, \boldsymbol{\alpha}_2) = \begin{pmatrix} 1 & 1 - \epsilon \\ 0 & \epsilon \end{pmatrix}$. It can be checked that $\{\boldsymbol{\alpha}_2^T \mathbf{X}_i\}_{i=1}^n$ is a strictly increasing sequence, so one can find a decreasing function f_2^* such that $f_2^*(\boldsymbol{\alpha}_2^T \mathbf{X}_i) = f_2(X_{i1})$ for every

$i = 1, \dots, n$. Consequently, by taking $\hat{f}^I(\mathbf{x}) = f_1(\mathbf{A}^T \mathbf{x}) + f_2^*(\mathbf{A}^T \mathbf{x}) + c$, we can ensure that $\hat{f}^I(\mathbf{X}_i) = Y_i$ for every $i = 1, \dots, n$.

We remark that this ‘perfect-fit’ phenomenon is quite general. Actually, one can show (via simple modifications of the above example) that it could happen whenever $\mathbf{L}_m \notin \mathcal{L}_m$, where $\mathcal{L}_m = \{1, \dots, 9\}$ when $m = 1$, and $\mathcal{L}_m = \{1, 4, 5, 6\}^m \cup \{1, 7, 8, 9\}^m$ when $m \geq 2$.

2. **Lack of upper semi-continuity of Λ_n .** The function $\Lambda_n(\cdot)$ need not be upper-semicontinuous, as illustrated by the following example:

Example 2. Again consider the Gaussian family with the identity link function. Take $d = 2$ and $\mathbf{L}_2 = (2, 2)^T$. Assume that there are $n = 4$ observations, namely, $\mathbf{X}_1 = (0, 0)^T$, $\mathbf{X}_2 = (0, 1)^T$, $\mathbf{X}_3 = (1, 0)^T$, $\mathbf{X}_4 = (1, 1)^T$, $Y_1 = Y_2 = Y_3 = 0$ and $Y_4 = 1$. If we take $\mathbf{A} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$, then it can be shown that $\Lambda_n(\mathbf{A}) = 3/32$ by fitting $\hat{f}^I(\mathbf{X}_1) = -\frac{1}{4}$, $\hat{f}^I(\mathbf{X}_2) = \hat{f}^I(\mathbf{X}_3) = 1/4$ and $\hat{f}^I(\mathbf{X}_4) = 3/4$. However, for any sufficiently small $\epsilon > 0$, if we define $\mathbf{A}_\epsilon = \begin{pmatrix} 1 - \epsilon & -\epsilon \\ -\epsilon & 1 - \epsilon \end{pmatrix}$, then we can take $\hat{f}^I(\mathbf{X}_i) = Y_i$ for $i = 1, \dots, 4$, so that $\Lambda_n(\mathbf{A}_\epsilon) = 1/8 > \Lambda_n(\mathbf{A})$.

This lack of upper semi-continuity means in general we cannot guarantee the existence of a maximiser.

As a result, certain modifications are required for our shape-constrained approach to be successful in the context of GAIMs. To deal with the first issue when $\mathbf{L}_m \notin \mathcal{L}_m$, we optimise $\Lambda_n(\cdot)$ over the subset of matrices

$$\mathcal{A}_d^{\mathbf{L}_m, \delta} = \{\mathbf{A} \in \mathcal{A}_d^{\mathbf{L}_m} : \lambda_{\min}(\mathbf{A}^T \mathbf{A}) \geq \delta\}$$

for some pre-determined $\delta > 0$, where $\lambda_{\min}(\cdot)$ denotes the smallest eigenvalue of a non-negative definite matrix. Other strategies are also possible. For example, when $\mathbf{L}_m = (2, \dots, 2)^T$, the ‘perfect-fit’ phenomenon can be avoided by only considering matrices that have the same signs in all entries (cf. Section 6.2 below).

To address the second issue, we will show that given $f_0^I \in \mathcal{G}_d^{\mathbf{L}_m}$ satisfying the identifiability conditions, to obtain a consistent estimator, it is sufficient to find \tilde{f}_n^I from the set

$$\tilde{\mathcal{S}}_n^{\mathbf{L}_m} \in \left\{ f^I : \mathbb{R}^d \rightarrow \mathbb{R} \mid f^I(\mathbf{x}) = f(\mathbf{A}^T \mathbf{x}), \text{ with } f \in \mathcal{F}^{\mathbf{L}_m}; \right. \quad (2)$$

$$\left. \begin{array}{l} \text{if } \mathbf{L}_m \in \mathcal{L}_m, \text{ then } \mathbf{A} \in \mathcal{A}_d^{\mathbf{L}_m}, \text{ otherwise, } \mathbf{A} \in \mathcal{A}_d^{\mathbf{L}_m, \delta}; \\ \bar{\ell}_{n,m}(f; (\mathbf{A}^T \mathbf{X}_1, Y_1), \dots, (\mathbf{A}^T \mathbf{X}_n, Y_n)) \geq \bar{\ell}_{n,m}(f_0; (\mathbf{A}_0^T \mathbf{X}_1, Y_1), \dots, (\mathbf{A}_0^T \mathbf{X}_n, Y_n)) \end{array} \right\},$$

for some $\delta \in (0, \lambda_{\min}(\mathbf{A}_0^T \mathbf{A}_0)]$. We write $\tilde{f}_n^I(\mathbf{x}) = \tilde{f}_n(\tilde{\mathbf{A}}_n^T \mathbf{x})$, where $\tilde{\mathbf{A}}_n = (\tilde{\alpha}_{n,1}, \dots, \tilde{\alpha}_{n,m}) \in \mathcal{A}_d^{\mathbf{L}_m}$ or $\mathcal{A}_d^{\mathbf{L}_m, \delta}$ is the estimated index matrix and $\tilde{f}_n(\mathbf{z}) = \sum_{j=1}^m \tilde{f}_{n,j}(z_j) + \tilde{c}_n$ is the estimated additive function satisfying $\tilde{f}_{n,j}(0) = 0$ for every $j = 1, \dots, m$. We call \tilde{f}_n^I the *shape-constrained additive index estimator* (SCAIE), and write $\tilde{\mathbf{A}}_n$ and $\tilde{f}_{n,1}, \dots, \tilde{f}_{n,m}$ respectively for the corresponding estimators of the index matrix and ridge functions.

When there exists a maximiser of the function $\Lambda_n(\cdot)$ over $\mathcal{A}_d^{\mathbf{L}_m}$ or $\mathcal{A}_d^{\mathbf{L}_m, \delta}$, the set $\tilde{S}_n^{\mathbf{L}_m}$ is non-empty; otherwise, a function satisfying (2) still exists in view of the following proposition:

Proposition 4. *The function $\Lambda_n(\cdot)$ is lower-semicontinuous.*

Note that if a maximiser of $\Lambda_n(\cdot)$ does not exist, there must exist some $\mathring{\mathbf{A}}_n$ such that $\Lambda_n(\mathring{\mathbf{A}}_n) > \Lambda_n(\mathbf{A}_0)$. It then follows from Proposition 4 that

$$\liminf_{\mathbf{A} \rightarrow \mathring{\mathbf{A}}_n} \Lambda_n(\mathbf{A}) \geq \Lambda_n(\mathring{\mathbf{A}}_n) > \Lambda_n(\mathbf{A}_0) \geq \bar{\ell}_{n,m}(f_0; (\mathbf{A}_0^T \mathbf{X}_1, Y_1) \dots, (\mathbf{A}_0^T \mathbf{X}_n, Y_n)),$$

so any \mathbf{A} sufficiently close to $\mathring{\mathbf{A}}_n$ yields a prediction function in $\tilde{S}_n^{\mathbf{L}_m}$. A stochastic search algorithm can be employed to find such matrices; see Section 4.2 for details.

3.3 Consistency of SCAIE

In this subsection, we show the consistency of \tilde{f}_n^I under a random design setting. In addition to (A.1) – (A.2), we require the following conditions:

- (B.2) The true prediction function f_0^I belongs to $\mathcal{G}_d^{\mathbf{L}_m}$.
- (B.3) Fix $\mathbf{L}_m \in \{1, 2, \dots, 9\}^m$. Suppose that $Y|\mathbf{X} \sim \text{EF}_{g,B}(g^{-1}(f_0^I(\mathbf{X})), \phi_0)$, where $\phi_0 \in (0, \infty)$ is the true dispersion parameter.
- (B.4) f_0^I is continuous on \mathbb{R}^d .
- (B.5) f_0^I and the corresponding index matrix \mathbf{A}_0 satisfy the identifiability conditions (B.1a) – (B.1f).

Theorem 5. *Assume (A.1) – (A.2) as well as (B.2) – (B.5). Then, provided $\delta \leq \lambda_{\min}(\mathbf{A}_0^T \mathbf{A}_0)$ when $\mathbf{L}_m \notin \mathcal{L}_m$, we have for every $a_0 \geq 0$ that*

$$\sup_{\tilde{f}_n^I \in \tilde{S}_n^{\mathbf{L}_m}} \sup_{\mathbf{x} \in [-a_0, a_0]^d} |\tilde{f}_n^I(\mathbf{x}) - f_0^I(\mathbf{x})| \xrightarrow{a.s.} 0, \quad \text{as } n \rightarrow \infty.$$

Consistency of the estimated index matrix and the ridge functions is established in the next corollary.

Corollary 6. Assume (A.1) – (A.2) and (B.2) – (B.5). Then, provided $\delta \leq \lambda_{\min}(\mathbf{A}_0^T \mathbf{A}_0)$ when $\mathbf{L}_m \notin \mathcal{L}_m$, we have for every $a_0 \geq 0$ that

$$\sup_{\tilde{f}_n^I \in \tilde{S}_n^{\mathbf{L}_m}} \min_{\tilde{\pi}_n \in \mathcal{P}_m} \left\{ \sum_{j=1}^m \|\tilde{\alpha}_{n, \tilde{\pi}_n(j)} - \alpha_{0,j}\|_1 + \sum_{j=1}^m \sup_{z_j \in [-a_0, a_0]} |\tilde{f}_{n, \tilde{\pi}_n(j)}(z_j) - f_{0,j}(z_j)| + |\tilde{c}_n - c_0| \right\} \xrightarrow{a.s.} 0,$$

as $n \rightarrow \infty$, where \mathcal{P}_m denotes the set of permutations of $\{1, \dots, m\}$.

Note that we can only hope to estimate the set of projection indices, and not their ordering (which is arbitrary). This explains why we take the minimum over all permutations of $\{1, \dots, m\}$ in Corollary 6 above.

4 Computational aspects

4.1 Computation of SCMLE

Throughout this subsection, we fix $\mathbf{L}_d = (l_1, \dots, l_d)^T$, the EF distribution and the values of the observations, and present an algorithm for computing SCMLE described in Section 2. We seek to reformulate the problem as convex program in terms of basis functions and apply an active set algorithm (Nocedal and Wright, 2006). Such algorithms have recently become popular for computing various shape-constrained estimators. For instance, Groeneboom, Jongbloed and Wellner (2008) used a version, which they called the ‘support reduction algorithm’ in the one-dimensional convex regression setting; Dümbgen and Rufibach (2011) applied another variant to compute the univariate log-concave maximum likelihood density estimator. Recently, Meyer (2013b) developed a ‘hinge’ algorithm for quadratic programming, which can also be viewed as a variant of the active set algorithm.

Without loss of generality, we assume in the following that only the first d_1 components ($d_1 \leq d$) of f_0 are linear, i.e. $l_1 = \dots = l_{d_1} = 1$ and $(l_{d_1+1}, \dots, l_d)^T \in \{2, \dots, 9\}^{d-d_1}$. Furthermore, we assume that the order statistics $\{X_{(i),j}\}_{i=1}^n$ of $\{X_{ij}\}_{i=1}^n$ are distinct for every $j = d - d_1 + 1, \dots, d$. Fix $\mathbf{x} = (x_1, \dots, x_d)^T \in \mathbb{R}^d$ and define the basis functions $g_{0j}(x_j) = x_j$ for $j = 1, \dots, d_1$ and, for

$i = 1, \dots, n,$

$$g_{ij}(x_j) = \begin{cases} \mathbb{1}_{\{X_{(i),j} \leq x_j\}} - \mathbb{1}_{\{X_{(i),j} \leq 0\}}, & \text{if } l_j = 2, \\ \mathbb{1}_{\{x_j < X_{(i),j}\}} - \mathbb{1}_{\{0 < X_{(i),j}\}}, & \text{if } l_j = 3, \\ (x_j - X_{(i),j})\mathbb{1}_{\{X_{(i),j} \leq x_j\}} + X_{(i),j}\mathbb{1}_{\{X_{(i),j} \leq 0\}}, & \text{if } l_j = 4 \text{ or } l_j = 5, \\ (X_{(i),j} - x_j)\mathbb{1}_{\{x_j \leq X_{(i),j}\}} - X_{(i),j}\mathbb{1}_{\{0 \leq X_{(i),j}\}}, & \text{if } l_j = 6, \\ (X_{(i),j} - x_j)\mathbb{1}_{\{X_{(i),j} \leq x_j\}} - X_{(i),j}\mathbb{1}_{\{X_{(i),j} \leq 0\}}, & \text{if } l_j = 7 \text{ or } l_j = 9, \\ (x_j - X_{(i),j})\mathbb{1}_{\{x_j \leq X_{(i),j}\}} + X_{(i),j}\mathbb{1}_{\{0 \leq X_{(i),j}\}}, & \text{if } l_j = 8. \end{cases}$$

Note that all the basis functions given above are zero at the origin. Let \mathcal{W} denote the set of weight vectors

$$\mathbf{w} = (w_{00}, w_{01}, \dots, w_{0d_1}, w_{1(d_1+1)}, \dots, w_{n(d_1+1)}, \dots, w_{1d}, \dots, w_{nd})^T \in \mathbb{R}^{n(d-d_1)+d_1+1}$$

satisfying

$$\begin{cases} w_{ij} \geq 0, & \text{for every } i = 1, \dots, n \text{ and every } j \text{ with } l_j \in \{2, 3, 5, 6, 8, 9\} \\ w_{ij} \geq 0, & \text{for every } i = 2, \dots, n \text{ and every } j \text{ with } l_j \in \{4, 7\}. \end{cases}$$

To compute SCMLE, it suffices to consider prediction functions of the form

$$f^{\mathbf{w}}(\mathbf{x}) = w_{00} + \sum_{j=1}^{d_1} w_{0j} g_{0j}(x_j) + \sum_{j=d_1+1}^d \sum_{i=1}^n w_{ij} g_{ij}(x_j)$$

subject to $\mathbf{w} \in \mathcal{W}$. Our optimisation problem can then be reformulated as maximising

$$\psi_n(\mathbf{w}) = \bar{\ell}_{n,d}(f^{\mathbf{w}}; (\mathbf{X}_1, Y_1), \dots, (\mathbf{X}_n, Y_n))$$

over $\mathbf{w} \in \mathcal{W}$. Note that ψ_n is a concave (but not necessarily strictly concave) function. Since

$$\sup_{\mathbf{w} \in \mathcal{W}} \bar{\ell}_{n,d}(f^{\mathbf{w}}) = \bar{\ell}_{n,d}(\hat{f}_n),$$

our goal here is to find a sequence $(\mathbf{w}^{(k)})$ such that $\psi_n(\mathbf{w}^{(k)}) \rightarrow \sup_{\mathbf{w} \in \mathcal{W}} \bar{\ell}_{n,d}(f^{\mathbf{w}})$ as $k \rightarrow \infty$. In Table 3, we give the pseudo-code for our active set algorithm for finding SCMLE, which is implemented in the R package `scar` (Chen and Samworth, 2014). We outline below some implementation details:

- (a) **IRLS**. Step 3 solves an unrestricted GLM problem by applying iteratively reweighted least squares (IRLS). Since the canonical link function is used here, IRLS is simply the Newton–Raphson method. If the EF distribution is Gaussian, then IRLS gives the exact solution of the

Step 1: Initialisation - outer loop: sort $\{X_i\}_{i=1}^n$ coordinate by coordinate; define the initial working set as $\mathcal{S}_1 = \{(0, j) | j \in \{1, \dots, d_1\}\} \cup \{(1, j) | l_j \in \{4, 7\}\}$; in addition, define the set of potential elements as

$$\mathcal{S} = \{(i, j) : i = 1, \dots, n, j = d_1 + 1, \dots, d\};$$

set the iteration count $k = 1$.

Step 2: Initialisation - inner loop: if $k > 1$, set $\mathbf{w}^* = \mathbf{w}^{(k-1)}$.

Step 3: Unrestricted generalised linear model (GLM): solve the following unrestricted GLM problem using iteratively reweighted least squares (IRLS):

$$\frac{1}{n} \sum_{h=1}^n \left\{ Y_h \left(\sum_{(i,j) \in \mathcal{S}_k} w_{ij} g_{ij}(X_{hj}) + w_{00} \right) - B \left(\sum_{(i,j) \in \mathcal{S}_k} w_{ij} g_{ij}(X_{hj}) + w_{00} \right) \right\},$$

where for $k > 1$, \mathbf{w}^* is used as a warm start. Store its solution in $\mathbf{w}^{(k)}$ (with zero weights for the elements outside \mathcal{S}_k).

Step 4: Working set refinement: if $k = 1$ or if $w_{ij} > 0$ for every $(i, j) \in \mathcal{S}_k \setminus \mathcal{S}_1$, go to **Step 5**; otherwise, define respectively the moving ratio p and the set of elements to drop as

$$p = \min_{\substack{(i,j) \in \mathcal{S}_k \setminus \mathcal{S}_1: \\ w_{ij} \leq 0}} \frac{w_{ij}^*}{w_{ij}^* - w_{ij}}, \quad \mathcal{S}_- = \left\{ (i, j) : (i, j) \in \mathcal{S}_k \setminus \mathcal{S}_1, w_{ij} \leq 0, \frac{w_{ij}^*}{w_{ij}^* - w_{ij}} = p \right\},$$

set $\mathcal{S}_k := \mathcal{S}_k \setminus \mathcal{S}_-$, overwrite \mathbf{w}^* by $\mathbf{w}^* := (1 - p)\mathbf{w}^* + p\mathbf{w}^{(k)}$ and go to **Step 3**.

Step 5: Derivative evaluation: for every $(i, j) \in \mathcal{S}$, compute $D_{i,j}^{(k)} = \frac{\partial \psi_n}{\partial w_{ij}}(\mathbf{w}^{(k)})$.

Step 6: Working set enlargement: write $\mathcal{S}_+ = \operatorname{argmax}_{(i,j) \in \mathcal{S}} D_{i,j}^{(k)}$ for the enlargement set, with maximum $D^{(k)} = \max_{(i,j) \in \mathcal{S}} D_{i,j}^{(k)}$; if $D^{(k)} \leq 0$ (or some other criteria are met if the EF distribution is non-Gaussian, e.g. $D^{(k)} < \epsilon_{IRLS}$ for some pre-determined small $\epsilon_{IRLS} > 0$), STOP the algorithm and go to **Step 7**; otherwise, pick any single-element subset $\mathcal{S}_+^* \subseteq \mathcal{S}_+$, let $\mathcal{S}_{k+1} = \mathcal{S}_k \cup \mathcal{S}_+^*$, set $k := k + 1$ and go back to **Step 2**.

Step 7: Output: for every $j = 1, \dots, d$, set $\hat{f}_{n,j}(x_j) = \sum_{\{(i,j) \in \mathcal{S}_k\}} w_{ij}^{(k)} g_{ij}(x_j)$; take $\hat{c}_n = w_{00}^{(k)}$; finally, return SCMLE as $\hat{f}_n(\mathbf{x}) = \sum_{j=1}^d \hat{f}_{n,j}(x_j) + \hat{c}_n$.

Table 3: Pseudo-code of the active set algorithm for computing SCMLE

problem in just one iteration. Otherwise, there is no closed-form expression for the solution, so a threshold ϵ_{IRLS} has to be picked to serve as part of the stopping criterion. Note that here IRLS can be replaced by other methods that solve GLM problems, though we found that IRLS offers competitive timing performance.

- (b) **Fast computation of the derivatives.** Although Step 5 appears at first sight to require $O(n^2d)$ operations, it can actually be completed with only $O(nd)$ operations by exploiting some nice recurrence relations. Define the ‘nominal’ residuals at the k -th iteration by

$$r_i^{(k)} = Y_i - \mu_i^{(k)}, \quad \text{for } i = 1, \dots, n,$$

where $\mu_i^{(k)} = g^{-1}(f^{\mathbf{w}^{(k)}}(\mathbf{X}_i))$ are the fitted mean values at the k -th iteration. Then

$$\frac{\partial \psi_n}{\partial w_{ij}}(\mathbf{w}^{(k)}) = \frac{1}{n} \sum_{u=1}^n r_u^{(k)} g_{ij}(X_{uj}).$$

For simplicity, we suppress henceforth the superscript k . Now fix j and reorder the pairs (r_i, X_{ij}) as $(r_{(1)}, X_{(1),j}), \dots, (r_{(n)}, X_{(n),j})$ such that $X_{(1),j} \leq \dots \leq X_{(n),j}$ (note that this is performed in Step 1). Furthermore, define

$$R_{i,j} = \begin{cases} \sum_{u=1}^i r_{(u)}, & \text{if } l_j \in \{2, 4, 5, 6\}, \\ -\sum_{u=1}^i r_{(u)}, & \text{if } l_j \in \{3, 7, 8, 9\}, \end{cases}$$

for $i = 1, \dots, n$, where we suppress the explicit dependence of $r_{(u)}$ on j in the notation. We have $R_{n,j} = 0$ due to the presence of the intercept w_{00} . The following recurrence relations can be derived by simple calculation:

- For $l_j \in \{2, 3\}$, we have $D_{1,j} = 0$ and $nD_{i,j} = -R_{i-1,j}$ for $i = 2, \dots, n$.
- For $l_j \in \{4, 5, 7, 9\}$, the initial condition is $D_{n,j} = 0$, and

$$nD_{i,j} = nD_{i+1,j} - R_{i,j} (X_{(i+1),j} - X_{(i),j}), \text{ for } i = n-1, \dots, 1.$$

- For $l_j \in \{6, 8\}$, the initial condition is $D_{1,j} = 0$, and

$$nD_{i,j} = nD_{i-1,j} + R_{i-1,j} (X_{(i),j} - X_{(i-1),j}), \text{ for } i = 2, \dots, n.$$

Therefore, the complexity of Step 5 in our implementation is $O(nd)$.

- (c) **Convergence.** If the EF distribution is Gaussian, then it follows from Theorem 1 of Groeneboom, Jongbloed and van der Vaart (2008) that our algorithm converges to the optimal solution after finitely many iterations. In general, the convergence of this active set strategy depends on two aspects:

- Convergence of IRLS. The convergence of Newton–Raphson method in Step 3 depends on the starting values. It is not guaranteed without step-size optimisation; cf. Jørgensen (1983). However, starting from the second iteration, each subsequent IRLS is performed by starting from the previous well-approximated solution, which typically makes the method work well.
- Accuracy of IRLS. If IRLS gives the *exact* solution every time, then $\psi_n(\mathbf{w}^{(k)})$ increases at each iteration. In particular, one can show that at the k -th iteration, the new element \mathcal{S}_+^* added into the working set in Step 6 will remain in the working set \mathcal{S}_{k+1} after the $(k+1)$ -th iteration. However, since IRLS only returns an approximate solution, there is no guarantee that the above-mentioned phenomenon continues to hold. One way to resolve this issue is to reduce the tolerance ϵ_{IRLS} if $\psi_n(\mathbf{w}^{(k)}) \leq \psi_n(\mathbf{w}^{(k-1)})$, and redo the computations for both the previous and the current iteration.

Here we terminate our algorithm in Step 6 if either $\psi_n(\mathbf{w}^{(k)})$ is non-increasing or $D^{(k)} < \epsilon_{IRLS}$. In our numerical work, we did not encounter convergence problems, even outside the Gaussian setting.

4.2 Computation of SCAIE

The computation of SCAIE can be divided into two parts:

1. For a given fixed A , find $f \in \text{cl}(\mathcal{F}^{\mathbf{L}_m})$ that maximises $\bar{\ell}_{n,m}(f; (\mathbf{A}^T \mathbf{X}_1, Y_1), \dots, (\mathbf{A}^T \mathbf{X}_n, Y_n))$ using the algorithm in Table 3 but with $\mathbf{A}^T \mathbf{X}_i$ replacing \mathbf{X}_i . Denote the corresponding maximum value by $\Lambda_n(\mathbf{A})$.
2. For a given lower-semicontinuous function Λ_n on $\mathcal{A}_d^{\mathbf{L}_m}$ or $\mathcal{A}_d^{\mathbf{L}_m, \delta}$ as appropriate, find a maximising sequence (\mathbf{A}^k) in this set.

The second part of this algorithm solves a finite-dimensional optimisation problem. Possible strategies include the differential evolution method (Price, Storn and Lampinen, 2005; Dümbgen, Samworth and Schuhmacher, 2011) or a stochastic search strategy (Dümbgen, Samworth and Schuhmacher, 2013) described below. In Table 4, we give the pseudo-code for computing SCAIE. We note that Step 4 of the stochastic search algorithm is parallelisable.

-
- Step 1: Initialisation:** let N denote the total number of stochastic searches; set $k = 1$.
- Step 2: Draw random matrices:** draw a $d \times m$ random matrix \mathbf{A}^k by initially choosing the entries to be independent and identically distributed $N(0, 1)$ random variables. For each column of \mathbf{A}^k , if there exists a $j \in \{1, \dots, m\}$ such that $l_j = 1$, subtract its projection to the j -th column of \mathbf{A}^k so that (B.1d) is satisfied, then normalise each column so (B.1b) and (B.1c) are satisfied.
- Step 3: Rejection sampling:** if $\mathbf{L}_m \notin \mathcal{L}_m$ and $\lambda_{\min}((\mathbf{A}^k)^T \mathbf{A}^k) < \delta$, then go back to **Step 2**; otherwise, if $k < N$, set $k := k + 1$ and go to **Step 2**.
- Step 4: Evaluation of Λ_n :** for every $k = 1, \dots, N$, compute $\Lambda_n(\mathbf{A}^k)$ using the active set algorithm described in Table 3.
- Step 5: Index matrix estimation - 1:** let $\mathbf{A}^* \in \arg\max_{1 \leq k \leq N} \Lambda_n(\mathbf{A}^k)$; set $\tilde{\mathbf{A}}_n = \mathbf{A}^*$;
- Step 6: Index matrix estimation - 2 (optional):** treat \mathbf{A}^* as a warm-start and apply another optimisation strategy to find \mathbf{A}^{**} in a neighbourhood of \mathbf{A}^* such that $\Lambda_n(\mathbf{A}^{**}) > \Lambda_n(\mathbf{A}^*)$; if such \mathbf{A}^{**} can be found, set $\tilde{\mathbf{A}}_n = \mathbf{A}^{**}$.
- Step 7: Output:** use the active set algorithm described in Table 3 to find

$$\tilde{f}_n \in \arg\max_{f \in \text{cl}(\mathcal{FL}_m)} \bar{\ell}_{n,m}(f; (\tilde{\mathbf{A}}_n^T \mathbf{X}_1, Y_1), \dots, (\tilde{\mathbf{A}}_n^T \mathbf{X}_n, Y_n));$$

finally, output SCAIE as $\tilde{f}_n^I(\mathbf{x}) = \tilde{f}_n(\tilde{\mathbf{A}}_n^T \mathbf{x})$.

Table 4: Pseudo-code of the stochastic search algorithm for computing SCAIE

5 Simulation study

To analyse the empirical performance of SCMLE and SCAIE, we ran a simulation study focusing on the running time and the predictive performance. Throughout this section, we took $\epsilon_{IRLS} = 10^{-8}$.

5.1 Generalised additive models with shape restrictions

We took $\mathbf{X}_1, \dots, \mathbf{X}_n \stackrel{\text{i.i.d.}}{\sim} U[-1, 1]^d$. The following three problems were considered:

1. Here $d = 4$. We set $\mathbf{L}_4 = (4, 4, 4, 4)^T$ and $f_0(\mathbf{x}) = |x_1| + |x_2| + |x_3|^3 + |x_4|^3$.
2. Here $d = 4$. We set $\mathbf{L}_4 = (5, 5, 5, 5)^T$ and

$$f_0(\mathbf{x}) = x_1 \mathbb{1}_{\{x_1 \geq 0\}} + x_2 \mathbb{1}_{\{x_2 \geq 0\}} + x_3^3 \mathbb{1}_{\{x_3 \geq 0\}} + x_4^3 \mathbb{1}_{\{x_4 \geq 0\}}.$$

3. Here $d = 8$. We set $\mathbf{L}_8 = (4, 4, 4, 4, 5, 5, 5, 5)^T$ and

$$f_0(\mathbf{x}) = |x_1| + |x_2| + |x_3|^3 + |x_4|^3 + x_5 \mathbb{1}_{\{x_5 \geq 0\}} + x_6 \mathbb{1}_{\{x_6 \geq 0\}} + x_7^3 \mathbb{1}_{\{x_7 \geq 0\}} + x_8^3 \mathbb{1}_{\{x_8 \geq 0\}}.$$

For each of these three problems, we considered three types of EF distributions:

- Gaussian: for $i = 1, \dots, n$, conditional on \mathbf{X}_i , draw independently $Y_i \sim N(f_0(\mathbf{X}_i), 0.5^2)$;
- Poisson: for $i = 1, \dots, n$, conditional on \mathbf{X}_i , draw independently $Y_i \sim \text{Pois}(g^{-1}(f_0(\mathbf{X}_i)))$, where $g(\mu) = \log \mu$;
- Binomial: for $i = 1, \dots, n$, draw N_i (independently of $\mathbf{X}_1, \dots, \mathbf{X}_n$) from a uniform distribution on $\{11, 12, \dots, 20\}$, and then draw independently $Y_i \sim N_i^{-1} \text{Bin}(N_i, g^{-1}(f(\mathbf{X}_i)))$, where $g(\mu) = \log \frac{\mu}{1-\mu}$.

Note that all of the component functions are convex, so f_0 is convex. This allows us to compare our method with other shape restricted methods in the Gaussian setting. Problem 3 represents a more challenging (higher-dimensional) problem. In the Gaussian setting, we compared the performance of SCMLE with Shape Constrained Additive Models (SCAM) (Pya and Wood, 2014), Generalised Additive Models with Integrated Smoothness estimation (GAMIS) (Wood, 2004), Multivariate Adaptive Regression Splines with maximum interaction degree equal to one (MARS) (Friedman, 1991), regression trees (Breiman *et al.*, 1984), Convex Adaptive Partitioning (CAP) (Hannah and Dunson, 2013), and Multivariate Convex Regression (MCR) (Lim and Glynn, 2012; Seijo and Sen, 2011). Some of the above-mentioned methods are not suitable to deal with non-identity link functions, so in the Poisson and Binomial settings, we only compared SCMLE with SCAM and GAMIS.

SCAM can be viewed as a shape-restricted version of GAMIS. It is implemented in the R package `scam` (Pya, 2012). GAMIS is implemented in the R package `mgcv` (Wood, 2012), while MARS can be founded in the R package `mda` (Hastie *et al.*, 2011). The method of regression trees is implemented in the R package `tree` (Ripley, 2012), and CAP is implemented in MATLAB by Hannah and Dunson (2013). We implemented MCR in MATLAB using the `interior-point-convex` solver. Default settings were used for all of the competitors mentioned above.

For different sample sizes $n = 200, 500, 1000, 2000, 5000$, we ran all the methods on 50 randomly generated datasets. Our numerical experiments were carried out on standard 32-bit desktops with 1.8 GHz CPUs. Each method was given at most one hour per dataset. Beyond this limit, the run was forced to stop and the corresponding results were omitted. Tables 13 and 14 in the online supplementary material provide the average running time of different methods per training dataset. Unsurprisingly SCMLE is slower than Tree or MARS, particularly in the higher-dimensional setting. On the other hand, it is typically faster than other shape-constrained methods such as SCAM and MCR. Note that MCR is particularly slow compared to the other methods, and becomes computationally infeasible for $n \geq 1000$.

To study the empirical performance of SCMLE, we drew 10^5 covariates independently from $U[-0.98, 0.98]^d$ and estimated the Mean Integrated Squared Error (MISE) $\mathbb{E} \int_{[-0.98, 0.98]^d} (\hat{f}_n - f_0)^2$ using Monte Carlo integration. Estimated MISEs are given in Tables 5 and 6. For every setting we considered, SCMLE performs better than Tree, CAP and MCR. This is largely due to the fact that these three estimators do not take into account the additive structure. In particular, MCR suffers severely from its boundary behaviour. It is also interesting to note that for small $n = 200$, SCAM and GAMIS occasionally offer slightly better performance than SCMLE. This is also mainly caused by the boundary behaviour of SCMLE, and is alleviated as the number of observations n increases. In each of the three problems considered, SCMLE enjoys better predictive performance than the other methods for $n \geq 500$. SCMLE appears to offer particular advantages when the true signal exhibits inhomogeneous smoothness, since it is able to regularise in a locally adaptive way, while both SCAM and GAMIS rely on a single level of regularisation throughout the covariate space.

5.2 Generalised additive index models with shape restrictions

In our comparisons of different estimators in GAIMs, we focused on the Gaussian case to facilitate comparisons with other methods. We took $\mathbf{X}_1, \dots, \mathbf{X}_n \stackrel{\text{i.i.d.}}{\sim} U[-1, 1]^d$, and considered the following two problems:

4. Here $d = 4$ and $m = 1$. We set $L_1 = 4$ and $f_0^I(\mathbf{x}) = |0.25x_1 + 0.25x_2 + 0.25x_3 + 0.25x_4|$.

Estimated MISEs: Gaussian

Problem 1

Method	$n = 200$	$n = 500$	$n = 1000$	$n = 2000$	$n = 5000$
SCMLE	0.413	0.167	0.085	0.044	0.021
SCAM	0.406	0.247	0.162	0.133	0.079
GAMIS	0.412	0.177	0.095	0.049	0.024
MARS	0.538	0.249	0.135	0.087	0.044
Tree	3.692	2.805	2.488	2.345	2.342
CAP	3.227	1.689	0.912	0.545	0.280
MCR	203.675	8415.607	-	-	-

Problem 2

Method	$n = 200$	$n = 500$	$n = 1000$	$n = 2000$	$n = 5000$
SCMLE	0.273	0.101	0.053	0.028	0.012
SCAM	0.264	0.107	0.058	0.032	0.016
GAMIS	0.363	0.154	0.079	0.041	0.019
MARS	0.417	0.177	0.087	0.050	0.021
Tree	1.995	1.277	1.108	1.015	0.973
CAP	1.282	0.742	0.415	0.251	0.145
MCR	940.002	14557.570	-	-	-

Problem 3

Method	$n = 200$	$n = 500$	$n = 1000$	$n = 2000$	$n = 5000$
SCMLE	11.023	3.825	2.096	1.107	0.479
SCAM	9.258	4.931	3.659	2.730	2.409
GAMIS	11.409	4.578	2.498	1.398	0.630
MARS	14.618	6.614	4.940	3.580	3.056
Tree	120.310	94.109	87.118	80.846	80.388
CAP	92.846	72.308	50.964	38.615	29.577
MCR	107.547	1535.022	-	-	-

Table 5: Estimated MISEs in the Gaussian setting for Problems 1, 2 and 3. The lowest MISE values are in bold font.

Estimated MISEs: Poisson and Binomial

Problem 1

Model	Method	$n = 200$	$n = 500$	$n = 1000$	$n = 2000$	$n = 5000$
Poisson	SCMLE	0.344	0.131	0.067	0.038	0.017
	SCAM	0.342	0.211	0.135	0.106	0.069
	GAMIS	0.330	0.142	0.078	0.043	0.021
Binomial	SCMLE	0.933	0.282	0.146	0.079	0.037
	SCAM	0.500	0.324	0.271	0.241	0.222
	GAMIS	0.639	0.284	0.153	0.085	0.040

Problem 2

Model	Method	$n = 200$	$n = 500$	$n = 1000$	$n = 2000$	$n = 5000$
Poisson	SCMLE	0.439	0.139	0.079	0.042	0.019
	SCAM	0.384	0.184	0.092	0.047	0.024
	GAMIS	0.505	0.210	0.121	0.064	0.030
Binomial	SCMLE	0.357	0.132	0.065	0.036	0.016
	SCAM	0.453	0.227	0.137	0.072	0.025
	GAMIS	0.449	0.173	0.090	0.054	0.024

Problem 3

Model	Method	$n = 200$	$n = 500$	$n = 1000$	$n = 2000$	$n = 5000$
Poisson	SCMLE	4.399	1.509	0.748	0.408	0.181
	SCAM	5.415	3.362	2.544	2.085	1.705
	GAMIS	4.698	1.949	0.981	0.571	0.275
Binomial	SCMLE	40.614	11.343	5.694	2.973	1.291
	SCAM	23.801	16.505	13.992	12.868	12.207
	GAMIS	25.439	11.908	6.317	3.516	1.551

Table 6: Estimated MISEs in the Poisson and Binomial settings for Problems 1, 2 and 3. The lowest MISE values are in bold font.

5. Here $d = 2$ and $m = 2$. We set $\mathbf{L}_2 = (4, 7)^T$ and $f_0^I(\mathbf{x}) = (0.5x_1 + 0.5x_2)^2 - |0.5x_1 - 0.5x_2|^3$.

In both problems, conditional on \mathbf{X}_i , we drew independently $Y_i \sim N(f_0^I(\mathbf{X}_i), 0.5^2)$ for $i = 1, \dots, n$.

We compared the performance of our SCAIE with Projection Pursuit Regression (PPR) (Friedman and Stuetzle, 1981), Multivariate Adaptive Regression Splines with maximum two interaction degrees (MARS) and regression trees (Tree). In addition, in Problem 4, we also considered the Semiparametric Single Index (SSI) method (Ichimura, 1993), CAP and MCR. SSI was implemented in the R package `np` (Hayfield and Racine, 2013). SCAIE was computed using the algorithm illustrated in Table 4. We picked the total number of stochastic searches to be $N = 100$. Note that because Problem 4 is a single-index problem (i.e. $m = 1$), there is no need to supply δ . In Problem 5, we chose $\delta = 0.1$. We considered sample sizes $n = 200, 500, 1000, 2000, 5000$.

Table 15 in the online supplementary material gives the average running time of different methods per training dataset. Although SCAIE is slower than PPR, MARS and Tree, its computation can be accomplished within a reasonable amount of time even when n is as large as 5000. As SSI adopts a leave-one-out cross-validation strategy, it is typically considerably slower than SCAIE.

Estimated MISEs of different estimators over $[-0.98, 0.98]^d$ are given in Table 7. In both Problems 4 and 5, we see that SCAIE outperforms its competitors for all the sample sizes we considered. It should, of course, be noted that SSI, PPR, MARS and Tree do not enforce the shape constraints, while MARS, Tree, CAP and MCR do not take into account the additive index structure.

In the index setting, it is also of interest to compare the performance of those methods that directly estimate the index matrix. We therefore estimated Root Mean Squared Errors (RMSEs), given by $\sqrt{\mathbb{E}\|\tilde{\boldsymbol{\alpha}}_{n,1} - \boldsymbol{\alpha}_{0,1}\|_2^2}$ in Problem 4, where $\boldsymbol{\alpha}_{0,1} = (0.25, 0.25, 0.25, 0.25)^T$. For Problem 5, we estimated mean errors in Amari distance ρ , defined by Amari *et al.* (1996) as

$$\rho(\tilde{\mathbf{A}}_n, \mathbf{A}_0) = \frac{1}{2d} \sum_{i=1}^d \left(\frac{\sum_{j=1}^d |C_{ij}|}{\max_{1 \leq j \leq d} |C_{ij}|} - 1 \right) + \frac{1}{2d} \sum_{j=1}^d \left(\frac{\sum_{i=1}^d |C_{ij}|}{\max_{1 \leq i \leq d} |C_{ij}|} - 1 \right),$$

where $C_{ij} = (\tilde{\mathbf{A}}_n \mathbf{A}_0^{-1})_{ij}$ and $\mathbf{A}_0 = \begin{pmatrix} 0.5 & 0.5 \\ 0.5 & -0.5 \end{pmatrix}$. This distance measure is invariant to permutation and takes values in $[0, d - 1]$. Results obtained for SCAIE and, where applicable, SSI and PPR, are displayed in Table 8. For both problems, SCAIE performs better in these senses than both SSI and PPR in terms of estimating the projection indices.

Estimated MISEs: Additive Index Models

Problem 4

Method	$n = 200$	$n = 500$	$n = 1000$	$n = 2000$	$n = 5000$
SCAIE	0.259	0.074	0.038	0.019	0.008
SSI	0.878	0.478	0.313	0.206	-
PPR	0.679	0.419	0.277	0.201	0.151
MARS	0.634	0.440	0.238	0.179	0.143
Tree	1.903	0.735	0.425	0.409	0.406
CAP	0.348	0.137	0.081	0.056	0.016
MCR	2539.912	35035.710	-	-	-

Problem 5

Method	$n = 200$	$n = 500$	$n = 1000$	$n = 2000$	$n = 5000$
SCAIE	0.078	0.030	0.016	0.008	0.005
PPR	0.137	0.055	0.027	0.015	0.010
MARS	0.081	0.034	0.018	0.010	0.006
Tree	0.366	0.241	0.266	0.310	0.309

Table 7: Estimated MISEs in Problems 4 and 5. The lowest MISE values are in bold font.

Problem 4: estimated RMSEs

Method	$n = 200$	$n = 500$	$n = 1000$	$n = 2000$	$n = 5000$
SCAIE	0.230	0.100	0.056	0.038	0.024
SSI	0.677	0.615	0.595	0.492	-
PPR	0.583	0.596	0.539	0.481	0.454

Problem 5: estimated Amari distance

Method	$n = 200$	$n = 500$	$n = 1000$	$n = 2000$	$n = 5000$
SCAIE	0.216	0.135	0.090	0.062	0.045
PPR	0.260	0.214	0.144	0.104	0.067

Table 8: Distance between the estimated index matrix and the truth: RMSEs were estimated in Problem 4, while the mean Amari errors were estimated in Problem 5. The lowest distances are in bold font.

6 Real data examples

In this section, we apply our estimators in two real data examples. In the first, we study doctoral publications in biochemistry and fit a generalised (Poisson) additive model with concavity constraints; while in the second, we use an additive index model with monotonicity constraints to study javelin performance in the decathlon.

6.1 Doctoral publications in biochemistry

The scientific productivity of a doctoral student may depend on many factors, including some or all of the number of young children they have, the productivity of the supervisor, their gender and marital status. Long (1990) studied this topic focusing on the gender difference; see also Long (1997). The dataset is available in the R package **AER** (Kleiber and Zeileis, 2013), and contains $n = 915$ observations. Here we model the number of articles written by the i -th PhD student in the last three years of their PhD as a Poisson random variable with mean μ_i , where

$$\log \mu_i = f_1(\mathbf{kids}_i) + f_2(\mathbf{mentor}_i) + a_3 \mathbf{gender}_i + a_4 \mathbf{married}_i + c,$$

for $i = 1, \dots, n$, where \mathbf{kids}_i and \mathbf{mentor}_i are respectively the number of that student’s children that are less than 6 years old, and the number of papers published by that student’s supervisor during the same period of time. Both \mathbf{gender}_i and $\mathbf{married}_i$ are factors taking values 0 and 1, where 1 indicates ‘female’ and ‘married’ respectively. In the original dataset, there is an extra continuous variable that measures the prestige of the graduate program. We chose to drop this variable in our example because: (i) its values were determined quite subjectively; and (ii) including this variable does not seem to improve the predictive power in the above settings.

To apply SCMLE, we assume that f_1 is a concave and monotone decreasing function, while f_2 is a concave function. The main estimates obtained from SCMLE are summarised in Table 9 and Figure 1. Outputs from SCAM and GAMIS are also reported for comparison. We see that with the exception of $\hat{f}_{n,2}$, estimates obtained from these methods are relatively close. Note that in Figure 1, the GAMIS estimate of f_2 displays local fluctuations that might be harder to interpret than the estimates obtained using SCMLE and SCAM.

Finally, we examine the prediction power of the different methods via cross-validation. Here we randomly split the dataset into training (70%) and validation (30%) subsets. For each split, we compute estimates using only the training set, and assess their predictive accuracy in terms of Root Mean Square Prediction Error (RMSPE) on the validation set. The reported RMSPEs in Table 10 are averages over 500 splits. Our findings suggest that whilst comparable to SCAM, SCMLE offers

Method	$\hat{f}_{n,1}(0)$	$\hat{f}_{n,1}(1)$	$\hat{f}_{n,1}(2)$	$\hat{f}_{n,1}(3)$	$\hat{a}_{n,3}$	$\hat{a}_{n,4}$
SCMLE	0	-0.110	-0.284	-0.816	-0.218	0.126
SCAM	0	-0.136	-0.303	-0.770	-0.224	0.152
GAMIS	0	-0.134	-0.301	-0.784	-0.226	0.157

Table 9: Estimates obtained from SCMLE, SCAM and GAMIS on the PhD publication dataset.

slight improvements over GAMIS and Tree for this dataset.

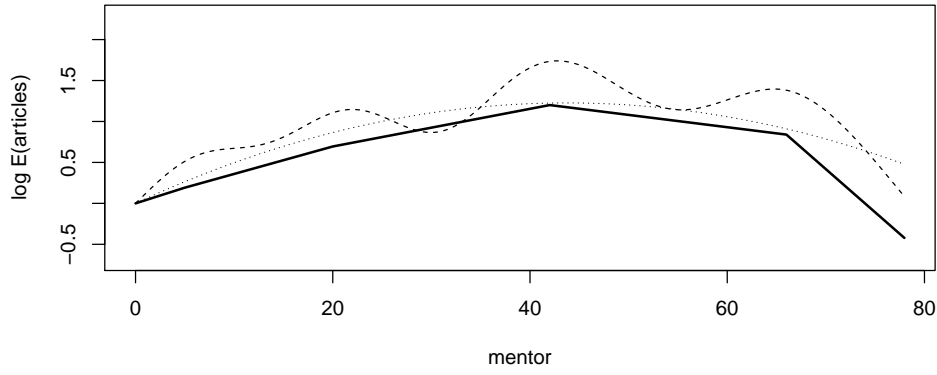


Figure 1: Different estimates of f_2 : SCMLE (solid), SCAM (dotted) and GAMIS (dashed).

Method	SCMLE	SCAM	GAMIS	Tree
RMSPE	1.822	1.823	1.838	1.890

Table 10: Estimated prediction errors of SCMLE, SCAM, GAMIS and Tree on the PhD publication dataset. The smallest RMSPE is in bold font.

6.2 Javelin throw

In this section, we consider the problem of predicting a decathlete’s javelin performance from their performances in the other decathlon disciplines. Our dataset consists of decathlon athletes who scored at least 6500 points in at least one athletic competition in 2012 and scored points in every event there. To avoid data dependency, we include only one performance from each athlete, namely their 2012 personal best (over the whole decathlon). The dataset, which consists of $n = 614$ observations, is available in the R package `scar` (Chen and Samworth, 2014). For simplicity, we only select events (apart from Javelin) that directly reflect the athlete’s ability in throwing and

short-distance running, namely, shot put, discus, 100 metres and 110 metres hurdles. We fit the following additive index model:

$$\begin{aligned} \text{javelin}_i &= f_1(A_{11} \text{100m}_i + A_{21} \text{110m}_i + A_{31} \text{shot}_i + A_{41} \text{discus}_i) \\ &\quad + f_2(A_{12} \text{100m}_i + A_{22} \text{110m}_i + A_{32} \text{shot}_i + A_{42} \text{discus}_i) + \epsilon_i, \end{aligned}$$

for $i = 1, \dots, 614$, where $\epsilon_i \stackrel{\text{i.i.d.}}{\sim} N(0, \sigma^2)$, and where javelin_i , 100m_i , 110m_i , shot_i and discus_i represent the corresponding decathlon event scores for the i -th athlete. For SCAIE, we assume that both f_1 and f_2 are monotone increasing, and also assume that $A_{11}, \dots, A_{41}, A_{12}, \dots, A_{42}$ are non-negative. This slightly restricted version of SCAIE aids interpretability of the indices, and prevents ‘perfect-fit’ phenomenon (cf. Section 3.2), so no choice of δ is required.

Table 11 gives the estimated index loadings by SCAIE. We observe that the first projection index can be interpreted as the general athleticism associated with the athlete, while the second can be viewed as a measure of throwing ability. Note that, when using SCAIE, $\hat{A}_{n,12}$ and $\hat{A}_{n,22}$ are relatively small. To further simplify our model, and to seek improvement in the prediction power, we therefore considered forcing these entries to be exactly zero in the optimisation steps of SCAIE. This sparse version is denoted as SCAIE_s. Its estimated index loadings are also reported in Table 11.

Method	$\hat{A}_{n,11}$	$\hat{A}_{n,21}$	$\hat{A}_{n,31}$	$\hat{A}_{n,41}$	$\hat{A}_{n,12}$	$\hat{A}_{n,22}$	$\hat{A}_{n,32}$	$\hat{A}_{n,42}$
SCAIE	0.262	0.343	0.222	0.173	0.006	0.015	0.522	0.457
SCAIE _s	0.235	0.305	0.140	0.320	0	0	0.536	0.464

Table 11: Estimated index loadings by SCAIE and SCAIE_s

To compare the performance of our methods with PPR, MARS with maximum two degrees of interaction and Tree, we again estimated the prediction power (in terms of RMSPE) via 500 repetitions of 70%/30% random splits into training/test sets. The corresponding RMSPEs are reported in Table 12. We see that both SCAIE and SCAIE_s outperform their competitors in this particular dataset. It is also interesting to note that SCAIE_s has a slightly lower RMSPE than SCAIE, suggesting that the simpler (sparser) model might be preferred for prediction here.

Method	SCAIE	SCAIE _s	PPR	MARS	Tree
RMSPE	81.276	80.976	82.898	82.915	85.085

Table 12: Estimated prediction errors of SCAIE, SCAIE_s, PPR, MARS and Tree on the decathlon dataset. The smallest RMSPE is in bold font.

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7 Appendix

PROOF OF PROPOSITION 1

Define the set

$$\Theta = \{\boldsymbol{\eta} = (\eta_1, \dots, \eta_n)^T \in \bar{\mathbb{R}}^n \mid \exists f \in \text{cl}(\mathcal{F}^{\mathbf{L}^d}) \text{ s.t. } \eta_i = f(\mathbf{X}_i), \forall i = 1, \dots, n\}.$$

We can rewrite the optimisation problem as finding $\hat{\boldsymbol{\eta}}_n$ such that

$$\hat{\boldsymbol{\eta}}_n \in \operatorname{argmax}_{\boldsymbol{\eta} \in \Theta} \bar{\ell}_n(\boldsymbol{\eta}),$$

where $\bar{\ell}_n(\boldsymbol{\eta}) = \frac{1}{n} \sum_{i=1}^n \ell_i(\eta_i)$, and where

$$\ell_i(\eta_i) = \begin{cases} Y_i \eta_i - B(\eta_i), & \text{if } \eta_i \in \text{dom}(B); \\ \lim_{a \rightarrow -\infty} Y_i a - B(a), & \text{if } \eta_i = -\infty; \\ \lim_{a \rightarrow \infty} Y_i a - B(a), & \text{if the EF is Gaussian, Poisson or Binomial, and } \eta_i = \infty; \\ -\infty, & \text{if the EF is Gamma and } \eta_i \in [0, \infty]. \end{cases}$$

Note that $\bar{\ell}_n$ is continuous on the non-empty set Θ and $\sup_{\boldsymbol{\eta} \in \Theta} \bar{\ell}_n(\boldsymbol{\eta})$ is finite. Moreover, by Lemma 9 in the online supplementary material, Θ is a closed subset of the compact set $\bar{\mathbb{R}}^n$, so is compact. It follows that $\bar{\ell}_n$ attains its maximum on Θ , so $\hat{S}_n^{\mathbf{L}^d} \neq \emptyset$.

To show the uniqueness of $\hat{\boldsymbol{\eta}}_n$, we now suppose that both $\boldsymbol{\eta}_1 = (\eta_{11}, \dots, \eta_{1n})^T$ and $\boldsymbol{\eta}_2 = (\eta_{21}, \dots, \eta_{2n})^T$ maximise $\bar{\ell}_n$. The only way we can have $\eta_{1i} = \infty$ is if the family is Binomial and $Y_i = 1$. But then $\ell_i(-\infty) = -\infty$, so we cannot have $\eta_{2i} = -\infty$. It follows that $\boldsymbol{\eta}_* = (\boldsymbol{\eta}_1 + \boldsymbol{\eta}_2)/2$ is well-defined, and $\boldsymbol{\eta}_* \in \Theta$, since Θ is convex. Now we can use the strict concavity of $\bar{\ell}_n$ on its domain to conclude that $\boldsymbol{\eta}_1 = \boldsymbol{\eta}_2 = \boldsymbol{\eta}_*$.

To prove Theorem 2, we require the following lemma, which says (roughly) that if any of the additive components (or the intercept) of $f \in \mathcal{F}^{\mathbf{L}^d}$ are large somewhere, then there is a non-trivial region on which either f is large, or a region on which $-f$ is large.

Lemma 7. Fix $a > 0$. There exists a finite collection \mathcal{C}_a of disjoint compact subsets of $[-2a, 2a]^d$ each having Lebesgue measure at least $(\frac{a}{2d})^d$, such that for any $f \stackrel{\mathcal{F}^{\mathbf{L}_d}}{\sim} (f_1, \dots, f_d, c)$,

$$\max_{C \in \mathcal{C}_a} \max \left\{ \inf_{\mathbf{x} \in C} f(\mathbf{x}), \inf_{\mathbf{x} \in C} -f(\mathbf{x}) \right\} \geq \frac{1}{4} \max \left\{ \sup_{|x_1| \leq a} |f_1(x_1)|, \dots, \sup_{|x_d| \leq a} |f_d(x_d)|, 2|c| \right\}.$$

Proof. Let $\max \{ \sup_{|x_1| \leq a} |f_1(x_1)|, \dots, \sup_{|x_d| \leq a} |f_d(x_d)|, 2|c| \} = M$ for some $M \geq 0$. Recalling that $f_1(0) = \dots = f_d(0) = 0$, and owing to the shape restrictions, this is equivalent to

$$\max \{ |f_1(-a)|, |f_1(a)|, \dots, |f_d(-a)|, |f_d(a)|, 2|c| \} = M.$$

We will prove the lemma by construction. For $j = 1, \dots, d$, consider the collection of intervals

$$\mathcal{D}_j = \begin{cases} \{ [-2a, -a], [a, 2a] \}, & \text{if } l_j \in \{2, 3, 5, 6, 8, 9\}; \\ \{ [-2a, -a], [-a/(4d), a/(4d)], [a, 2a] \}, & \text{if } l_j \in \{1, 4, 7\}. \end{cases}$$

Let $\mathcal{C}_a = \{ \times_{j=1}^d D_j : D_j \in \mathcal{D}_j \}$, so that $|\mathcal{C}_a| \leq 3^d$. The two cases below validate our construction:

1. $\max \{ |f_1(-a)|, |f_1(a)|, \dots, |f_d(-a)|, |f_d(a)| \} < M$. Then it must be the case that $|c| = M/2$ and, without loss of generality, we may assume $c = M/2$. For $j = 1, \dots, d$, if $l_j \in \{2, 3, 5, 6, 8, 9\}$, then due to the monotonicity and the fact that $f_j(0) = 0$, either

$$\inf_{x_j \in [-2a, -a]} f_j(x_j) \geq 0 \quad \text{or} \quad \inf_{x_j \in [a, 2a]} f_j(x_j) \geq 0.$$

For $l_j \in \{1, 4, 7\}$, by the convexity/concavity, $\sup_{x_j \in [-a/(4d), a/(4d)]} |f_j(x_j)| \leq M/(4d)$. Hence

$$\max_{C \in \mathcal{C}_a} \inf_{\mathbf{x} \in C} f(\mathbf{x}) \geq -dM/(4d) + M/2 = M/4.$$

2. $\max \{ |f_1(-a)|, |f_1(a)|, \dots, |f_d(-a)|, |f_d(a)| \} = M$ and $|c| \leq M/2$. Without loss of generality, we may assume that $f_1(-a) = M$. Since $f_1(0) = 0$ and $|f_1(a)| \leq M$, we can assume $l_1 \in \{1, 3, 4, 6\}$.

Therefore, $\inf_{x_1 \in [-2a, -a]} f_1(x_1) = M$. Let

$$D_j = \begin{cases} [-a/(4d), a/(4d)], & \text{if } l_j \in \{1, 4, 7\} \\ [a, 2a], & \text{if } l_j \in \{2, 5, 8\} \\ [-2a, -a], & \text{if } l_j \in \{3, 6, 9\} \end{cases}$$

for $j = 2, \dots, d$. Now for $C = [-2a, -a] \times \times_{j=2}^d D_j$, we have

$$\inf_{\mathbf{x} \in C} f(\mathbf{x}) \geq M - (d-1)M/(4d) - M/2 \geq M/4.$$

□

PROOF OF THEOREM 2

For convenience, we first present the proof of consistency in the case where the EF distribution is Binomial. Consistency for the other EF distributions listed in Table 2 can be established using essentially the same proof structure with some minor modifications. We briefly outline these changes at the end of the proof. Our proof can be divided into five steps.

Step 1: Lower bound for the scaled partial log-likelihood. It follows from Assumption (A.1) and the strong law of large numbers that

$$\liminf_{n \rightarrow \infty} \sup_{f \in \text{cl}(\mathcal{F}^{\mathbf{L}_d})} \bar{\ell}_n(f) \geq \lim_{n \rightarrow \infty} \bar{\ell}_n(f_0) = \mathbb{E}\{g^{-1}(f_0(\mathbf{X}))f_0(\mathbf{X}) - B(f_0(\mathbf{X}))\} =: \bar{L}_0$$

almost surely.

Step 2: Bounding $|\hat{f}_n|$ on $[-a, a]^d$ for any fixed $a > 0$. For $M > 0$, let

$$\mathcal{F}_{a,M}^{\mathbf{L}_d} = \left\{ f \stackrel{\mathcal{F}^{\mathbf{L}_d}}{\sim} (f_1, \dots, f_d, c) : \max\{|f_1(-a)|, |f_1(a)|, \dots, |f_d(-a)|, |f_d(a)|, 2|c|\} \leq M \right\}. \quad (3)$$

We will prove that there exists a deterministic constant $M = M(a) \in (0, \infty)$ such that, with probability one, we have $\hat{S}_n^{\mathbf{L}_d} \subseteq \text{cl}(\mathcal{F}_{a,M(a)}^{\mathbf{L}_d})$ for sufficiently large n . To this end, let $\mathcal{C}_a = \{C_1, \dots, C_N\}$ be the finite collection of compact subsets of $[-2a, 2a]^d$ constructed in the proof of Lemma 7, and set

$$M = 4B^{-1} \left(\frac{-\bar{L}_0 + 1}{\min_{1 \leq k \leq N, t \in \{0,1\}} \mathbb{P}(\mathbf{X} \in C_k, Y = t)} \right).$$

Note that

$$\begin{aligned} & \limsup_{n \rightarrow \infty} \sup_{f \in \text{cl}(\mathcal{F}^{\mathbf{L}_d} \setminus \mathcal{F}_{a,M}^{\mathbf{L}_d})} \bar{\ell}_n(f) \\ & \leq \max_{1 \leq k \leq N} \limsup_{n \rightarrow \infty} \sup_{f \in \text{cl}(\mathcal{F}^{\mathbf{L}_d} \setminus \mathcal{F}_{a,M}^{\mathbf{L}_d})} \frac{1}{n} \sum_{i=1}^n \{Y_i f(\mathbf{X}_i) - B(f(\mathbf{X}_i))\} \mathbb{1}_{\{\mathbf{X}_i \notin C_k \cup Y_i \notin \{0,1\}\}} \end{aligned} \quad (4)$$

$$+ \min_{1 \leq k \leq N} \limsup_{n \rightarrow \infty} \sup_{f \in \text{cl}(\mathcal{F}^{\mathbf{L}_d} \setminus \mathcal{F}_{a,M}^{\mathbf{L}_d})} \frac{1}{n} \sum_{i=1}^n \{Y_i f(\mathbf{X}_i) - B(f(\mathbf{X}_i))\} \mathbb{1}_{\{\mathbf{X}_i \in C_k \cap Y_i \in \{0,1\}\}}. \quad (5)$$

Now (4) is non-positive, since $Y_i \eta - B(\eta) = Y_i \eta - \log(1 + e^\eta) \leq 0$ for all $\eta \in \bar{\mathbb{R}}$ and $Y_i \in \{0, 1/T, 2/T, \dots, 1\}$. We now claim that the supremum over $f \in \text{cl}(\mathcal{F}^{\mathbf{L}_d} \setminus \mathcal{F}_{a,M}^{\mathbf{L}_d})$ in (5) can be replaced with a supremum over $f \in \mathcal{F}^{\mathbf{L}_d} \setminus \mathcal{F}_{a,M}^{\mathbf{L}_d}$. To see this, let

$$\Theta_0 = \{\boldsymbol{\eta} = (\eta_1, \dots, \eta_n)^T \in \bar{\mathbb{R}}^n : \exists f \in \text{cl}(\mathcal{F}^{\mathbf{L}_d} \setminus \mathcal{F}_{a,M}^{\mathbf{L}_d}) \text{ s.t. } \eta_i = f(\mathbf{X}_i), \forall i = 1, \dots, n\}.$$

Suppose that $(\boldsymbol{\eta}^m) \in \Theta_0$ is such that the corresponding $(f^m) \in \text{cl}(\mathcal{F}^{\mathbf{L}_d} \setminus \mathcal{F}_{a,M}^{\mathbf{L}_d})$ is a maximising

sequence in the sense that

$$\frac{1}{n} \sum_{i=1}^n \{Y_i f^m(\mathbf{X}_i) - B(f^m(\mathbf{X}_i))\} \mathbb{1}_{\{\mathbf{X}_i \in C_k \cap Y_i \in \{0,1\}\}} \nearrow \sup_{f \in \text{cl}(\mathcal{F}^{\mathbf{L}_d} \setminus \mathcal{F}_{a,M}^{\mathbf{L}_d})} \frac{1}{n} \sum_{i=1}^n \{Y_i f(\mathbf{X}_i) - B(f(\mathbf{X}_i))\} \mathbb{1}_{\{\mathbf{X}_i \in C_k \cap Y_i \in \{0,1\}\}}.$$

By reducing to a subsequence if necessary, we may assume $\boldsymbol{\eta}^m \rightarrow \boldsymbol{\eta}^0$, say, as $m \rightarrow \infty$, where $\boldsymbol{\eta}^0 = (\eta_1^0, \dots, \eta_n^0)^T \in \bar{\mathbb{R}}^n$. Since, for each $m \in \mathbb{N}$, we can find a sequence $(f^{m,k})_k \in \mathcal{F}^{\mathbf{L}_d} \setminus \mathcal{F}_{a,M}^{\mathbf{L}_d}$ such that $f^{m,k} \rightarrow f^m$ pointwise in $\bar{\mathbb{R}}$ as $k \rightarrow \infty$, it follows that we can pick $k_m \in \mathbb{N}$ such that $f^{m,k_m}(\mathbf{X}_i) \rightarrow \eta_i^0$ as $m \rightarrow \infty$, for all $i = 1, \dots, n$. Moreover, $(\eta_1, \dots, \eta_n) \mapsto \frac{1}{n} \sum_{i=1}^n \{Y_i \eta_i - B(\eta_i)\} \mathbb{1}_{\{\mathbf{X}_i \in C_k \cap Y_i \in \{0,1\}\}}$ is continuous on $\bar{\mathbb{R}}^n$, and we deduce that $(f^{m,k_m}) \in \mathcal{F}^{\mathbf{L}_d} \setminus \mathcal{F}_{a,M}^{\mathbf{L}_d}$ is also a maximising sequence, which establishes our claim.

Recall that by Lemma 7, for any $f \in \mathcal{F}^{\mathbf{L}_d} \setminus \mathcal{F}_{a,M}^{\mathbf{L}_d}$, we can always find $C_{k^*} \in \mathcal{C}_a$ such that

$$\max \left\{ \inf_{\mathbf{x} \in C_{k^*}} f(\mathbf{x}), \inf_{\mathbf{x} \in C_{k^*}} -f(\mathbf{x}) \right\} \geq M/4.$$

Combining the non-positivity of (4) and our argument above removing the closure in (5), we deduce by the strong law of large numbers that

$$\begin{aligned} & \limsup_{n \rightarrow \infty} \sup_{f \in \text{cl}(\mathcal{F}^{\mathbf{L}_d} \setminus \mathcal{F}_{a,M}^{\mathbf{L}_d})} \bar{\ell}_n(f) \\ & \leq \max \left\{ -B(M/4) \mathbb{P}(\mathbf{X} \in C_{k^*}, Y = 0), \{-M/4 - B(-M/4)\} \mathbb{P}(\mathbf{X} \in C_{k^*}, Y = 1) \right\} \\ & \leq - \min_{1 \leq k \leq N, t \in \{0,1\}} \mathbb{P}(\mathbf{X} \in C_k, Y = t) B(M/4) = \bar{L}_0 - 1, \end{aligned}$$

where, we have used the property that $B(t) = t + B(-t)$ for the penultimate inequality, and the definition of M for the final equality. Comparing this bound with the result of Step 1, we deduce that $\hat{S}_n^{\mathbf{L}_d} \cap \text{cl}(\mathcal{F}^{\mathbf{L}_d} \setminus \mathcal{F}_{a,M}^{\mathbf{L}_d}) = \emptyset$ for sufficiently large n , almost surely. But it is straightforward to check that $\text{cl}(\mathcal{F}^{\mathbf{L}_d}) = \text{cl}(\mathcal{F}_{a,M}^{\mathbf{L}_d}) \cup \text{cl}(\mathcal{F}^{\mathbf{L}_d} \setminus \mathcal{F}_{a,M}^{\mathbf{L}_d})$, and the result follows.

Step 3: Lipschitz constant for the convex/concave components of \hat{f}_n on $[-a, a]$. For $M_1, M_2 > 0$, let

$$\mathcal{F}_{a,M_1,M_2}^{\mathbf{L}_d} = \left\{ f \stackrel{\mathcal{F}^{\mathbf{L}_d}}{\sim} (f_1, \dots, f_d, c) \in \mathcal{F}_{a,M_1}^{\mathbf{L}_d} : |f_j(z_1) - f_j(z_2)| \leq M_2 |z_1 - z_2|, \forall z_1, z_2 \in [-a, a], \right. \\ \left. \forall j \text{ with } l_j \in \{1, 4, 5, 6, 7, 8, 9\} \right\}.$$

For notational convenience, we define $W(a) = M(a) + M(a+1) + 1$. By Lemma 10 in the online supplementary material,

$$\text{cl}(\mathcal{F}_{a,M(a)}^{\mathbf{L}_d}) \cap \text{cl}(\mathcal{F}_{a+1,M(a+1)}^{\mathbf{L}_d}) \subseteq \text{cl}(\mathcal{F}_{a,M(a),W(a)}^{\mathbf{L}_d}).$$

From this and the result of Step 2, we have that for any fixed $a > 0$, with probability one, $\hat{S}_n^{\mathbf{L}^d} \subseteq \text{cl}(\mathcal{F}_{a,M(a),W(a)}^{\mathbf{L}^d})$ for sufficiently large n .

Step 4: Glivenko–Cantelli Classes.

For, $a > 0$, $M_1 > 0$, $M_2 > 0$ and $j = 1, \dots, d$, let

$$\check{\mathcal{F}}_{a,M_1,M_2}^{\mathbf{L}^d} = \left\{ \check{f} : \mathbb{R}^d \rightarrow \mathbb{R} \mid \check{f}(\mathbf{x}) = f(\mathbf{x}) \mathbb{1}_{\{\mathbf{x} \in [-a,a]^d\}}, f \in \mathcal{F}_{a,M_1,M_2}^{\mathbf{L}^d} \right\}$$

and

$$(\check{\mathcal{F}}_{a,M_1,M_2}^{\mathbf{L}^d})_j = \left\{ \check{f} : \mathbb{R}^d \rightarrow \mathbb{R} \mid \check{f}(\mathbf{x}) = f_j(x_j) \mathbb{1}_{\{\mathbf{x} \in [-a,a]^d\}} \text{ for some } f \stackrel{\mathcal{F}^{\mathbf{L}^d}}{\sim} (f_1, \dots, f_d, c) \in \mathcal{F}_{a,M_1,M_2}^{\mathbf{L}^d} \right\}.$$

We first claim that each $(\check{\mathcal{F}}_{a,M_1,M_2}^{\mathbf{L}^d})_j$ is a $P_{\mathbf{X}}$ -Glivenko–Cantelli class, where $P_{\mathbf{X}}$ is the distribution of \mathbf{X} . To see this, note that by Theorem 2.7.5 of van der Vaart and Wellner (1996), there exists a universal constant $C > 0$ and functions $g_k^L, g_k^U : \mathbb{R} \rightarrow [0, 1]$ for $k = 1, \dots, N_1$ with $N_1 = e^{2M_1 C/\epsilon}$ such that $\mathbb{E}|g_k^U(X_{1j}) - g_k^L(X_{1j})| \leq \epsilon/(2M_1)$ and such that for every monotone function $g : \mathbb{R} \rightarrow [0, 1]$, we can find $k^* \in \{1, \dots, N_1\}$ with $g_{k^*}^L \leq g \leq g_{k^*}^U$. By Corollary 2.7.10, the same property holds for convex or concave functions from $[-a, a]$ to $[0, 1]$, provided we use N_2 brackets, where $N_2 = \exp\{C(1 + \frac{M_2}{2M_1})^{1/2}(2M_1/\epsilon)^{1/2}\}$. It follows that if j corresponds to a monotone component, then the class of functions

$$\tilde{g}_k^L(x) = 2M_1(g_k^L(x_j) - 1/2) \mathbb{1}_{\{\mathbf{x} \in [-a,a]^d\}}, \quad \tilde{g}_k^U(x) = 2M_1(g_k^U(x_j) - 1/2) \mathbb{1}_{\{\mathbf{x} \in [-a,a]^d\}},$$

for $k = 1, \dots, N_1$, forms an ϵ -bracketing set for $(\check{\mathcal{F}}_{a,M_1,M_2}^{\mathbf{L}^d})_j$ in the $L_1(P_{\mathbf{X}})$ -norm. Similarly, if j corresponds to a convex or concave component, we can define in the same way an ϵ -bracketing set for $(\check{\mathcal{F}}_{a,M_1,M_2}^{\mathbf{L}^d})_j$ of cardinality N_2 for $(\check{\mathcal{F}}_{a,M_1,M_2}^{\mathbf{L}^d})_j$. We deduce by Theorem 2.4.1 of van der Vaart and Wellner (1996) that each $(\check{\mathcal{F}}_{a,M_1,M_2}^{\mathbf{L}^d})_j$ is a $P_{\mathbf{X}}$ -Glivenko–Cantelli class. But then

$$\sup_{\check{f} \in \check{\mathcal{F}}_{a,M_1,M_2}^{\mathbf{L}^d}} \left| \frac{1}{n} \sum_{i=1}^n \check{f}(\mathbf{X}_i) - \mathbb{E} \check{f}(\mathbf{X}) \right| \leq \sum_{j=1}^d \sup_{\check{f}_j \in (\check{\mathcal{F}}_{a,M_1,M_2}^{\mathbf{L}^d})_j} \left| \frac{1}{n} \sum_{i=1}^n \check{f}_j(X_{ij}) - \mathbb{E} \check{f}_j(X_{1j}) \right|,$$

so $\check{\mathcal{F}}_{a,M_1,M_2}^{\mathbf{L}^d}$ is $P_{\mathbf{X}}$ -Glivenko–Cantelli. We now use this fact to show that the class of functions

$$\mathcal{H}_{a,M_1,M_2} = \left\{ h_f : \mathbb{R}^d \times \mathbb{R} \rightarrow \mathbb{R} \mid h_f(\mathbf{x}, y) = \{y f(\mathbf{x}) - B(f(\mathbf{x}))\} \mathbb{1}_{\{\mathbf{x} \in [-a,a]^d\}}, f \in \mathcal{F}_{a,M_1,M_2}^{\mathbf{L}^d} \right\}$$

is P -Glivenko–Cantelli, where P is the distribution of (\mathbf{X}, Y) . Define $f^*, f^{**} : \mathbb{R}^d \times \mathbb{R} \rightarrow \mathbb{R}$ by $f^*(\mathbf{x}, y) = y$ and $f^{**}(\mathbf{x}, y) = \mathbb{1}_{\{\mathbf{x} \in [-a,a]^d\}}$. Let

$$\mathcal{F}_1 = \{ f : \mathbb{R}^d \times \mathbb{R} \rightarrow \mathbb{R} \mid f(\mathbf{x}, y) = \check{f}(\mathbf{x}), \check{f} \in \check{\mathcal{F}}_{a,M_1,M_2}^{\mathbf{L}^d} \},$$

let $\mathcal{F}_2 = \{f^*\}$ and let $\mathcal{F}_3 = \{f^{**}\}$; finally define $\psi : \mathbb{R} \times \mathbb{R} \times \mathbb{R} \rightarrow \mathbb{R}$ by $\psi(u, v, w) = \{vu - B(u)\}w$. Then $\mathcal{H} = \psi(\mathcal{F}_1, \mathcal{F}_2, \mathcal{F}_3)$, where

$$\psi(\mathcal{F}_1, \mathcal{F}_2, \mathcal{F}_3) = \{\psi(f_1(\mathbf{x}, y), f_2(\mathbf{x}, y), f_3(\mathbf{x}, y)) : f_1 \in \mathcal{F}_1, f_2 \in \mathcal{F}_2, f_3 \in \mathcal{F}_3\}.$$

Now $\mathcal{F}_1, \mathcal{F}_2$ and \mathcal{F}_3 are P -Glivenko–Cantelli, ψ is continuous and (recalling that $|Y| \leq 1$ in the Binomial setting),

$$\sup_{f_1 \in \mathcal{F}_1} \sup_{f_2 \in \mathcal{F}_2} \sup_{f_3 \in \mathcal{F}_3} |\psi(f_1(\mathbf{x}, y), f_2(\mathbf{x}, y), f_3(\mathbf{x}, y))| \leq M_1(d+1) + B(M_1(d+1)),$$

which is P -integrable. We deduce from Theorem 3 of van der Vaart and Wellner (2000) that $\mathcal{H}_{a, M_1, M_2}$ is P -Glivenko–Cantelli.

Step 5: Almost sure convergence of \hat{f}_n . For $\epsilon > 0$, let

$$B_\epsilon(f_0) = \left\{ f : \mathbb{R}^d \rightarrow \mathbb{R} \left| \sup_{\mathbf{x} \in [-a_0, a_0]^d} |f(\mathbf{x}) - f_0(\mathbf{x})| \leq \epsilon \right. \right\},$$

where we suppress the dependence of $B_\epsilon(f_0)$ on a_0 in the notation. Our aim to show that with probability 1, we have $\hat{S}_n^{\mathbf{L}^d} \cap \text{cl}(\mathcal{F}^{\mathbf{L}^d} \setminus B_\epsilon(f_0)) = \emptyset$ for sufficiently large n . In Lemma 11 in the online supplementary material, it is established that for any $\epsilon > 0$,

$$\begin{aligned} \zeta(a^*) &:= \mathbb{E}[\{Y f_0(\mathbf{X}) - B(f_0(\mathbf{X}))\} \mathbb{1}_{\{\mathbf{X} \in [-a^*, a^*]^d\}}] \\ &\quad - \sup_{f \in \mathcal{F}_{a_0, M(a_0), W(a_0)}^{\mathbf{L}^d} \setminus B_\epsilon(f_0)} \mathbb{E}[\{Y f(\mathbf{X}) - B(f(\mathbf{X}))\} \mathbb{1}_{\{\mathbf{X} \in [-a^*, a^*]^d\}}] \end{aligned} \quad (6)$$

is positive and a non-decreasing function of $a^* > a_0 + 1$. Since we also have that (in the Binomial setting), $-\log 2 \leq g^{-1}(t)t - B(t) \leq 0$, we can therefore choose $a^* > a_0 + 1$ such that

$$|\mathbb{E}[\{Y f_0(\mathbf{X}) - B(f_0(\mathbf{X}))\} \mathbb{1}_{\{\mathbf{X} \notin [-a^*, a^*]^d\}}]| \leq \zeta(a^*)/3. \quad (7)$$

Let

$$\begin{aligned} \mathcal{F}^* &= \text{cl}(\mathcal{F}_{a_0, M(a_0)}^{\mathbf{L}^d} \setminus B_\epsilon(f_0)) \cap \text{cl}(\mathcal{F}_{a_0+1, M(a_0+1)}^{\mathbf{L}^d} \setminus B_\epsilon(f_0)) \\ &\quad \cap \text{cl}(\mathcal{F}_{a^*, M(a^*)}^{\mathbf{L}^d} \setminus B_\epsilon(f_0)) \cap \text{cl}(\mathcal{F}_{a^*+1, M(a^*+1)}^{\mathbf{L}^d} \setminus B_\epsilon(f_0)). \end{aligned}$$

Observe that by the result of Step 2, we have that with probability one, $\hat{S}_n^{\mathbf{L}^d} \subseteq \mathcal{F}^* \cup \text{cl}(B_\epsilon(f_0))$ for sufficiently large n . By Lemma 12 in the online supplementary material,

$$\begin{aligned} &\left\{ \sup_{f \in \mathcal{F}^*} \frac{1}{n} \sum_{i=1}^n \{Y_i f(\mathbf{X}_i) - B(f(\mathbf{X}_i))\} \geq \bar{L}_0 - \zeta(a^*)/3 \right\} \\ &\subseteq \left\{ \sup_{f \in (\mathcal{F}_{a_0, M(a_0), W(a_0)}^{\mathbf{L}^d} \cap \mathcal{F}_{a^*, M(a^*)+1, W(a^*)+1}^{\mathbf{L}^d}) \setminus B_\epsilon(f_0)} \frac{1}{n} \sum_{i=1}^n \{Y_i f(\mathbf{X}_i) - B(f(\mathbf{X}_i))\} \mathbb{1}_{\{\mathbf{X}_i \in [-a^*, a^*]^d\}} \right. \\ &\quad \left. + \sup_{f \in \mathcal{F}^{\mathbf{L}^d}} \frac{1}{n} \sum_{i=1}^n \{Y_i f(\mathbf{X}_i) - B(f(\mathbf{X}_i))\} \mathbb{1}_{\{\mathbf{X}_i \notin [-a^*, a^*]^d\}} \geq \bar{L}_0 - \zeta(a^*)/3 \right\}, \end{aligned} \quad (8)$$

Here the closure operator in (8) can be dropped by the same argument as in Step 2. Now note that

$$\left\{ h_f : \mathbb{R}^d \times \mathbb{R} \rightarrow \mathbb{R} \mid h_f(\mathbf{x}, y) = \{yf(\mathbf{x}) - B(f(\mathbf{x}))\} \mathbb{1}_{\{\mathbf{x} \in [-a^*, a^*]^d\}}, \right. \\ \left. f \in (\mathcal{F}_{a_0, M(a_0), W(a_0)}^{\mathbf{L}_d} \cap \mathcal{F}_{a^*, M(a^*)+1, W(a^*)+1}^{\mathbf{L}_d}) \setminus B_\epsilon(f_0) \right\} \subseteq \mathcal{H}_{a^*, M(a^*)+1, W(a^*)+1},$$

so the class is P -Glivenko–Cantelli, by the result of Step 4. We therefore have that with probability one,

$$\begin{aligned} \limsup_{n \rightarrow \infty} \sup_{f \in (\mathcal{F}_{a_0, M(a_0), W(a_0)}^{\mathbf{L}_d} \cap \mathcal{F}_{a^*, M(a^*)+1, W(a^*)+1}^{\mathbf{L}_d}) \setminus B_\epsilon(f_0)} \frac{1}{n} \sum_{i=1}^n \{Y_i f(\mathbf{X}_i) - B(f(\mathbf{X}_i))\} \mathbb{1}_{\{\mathbf{X}_i \in [-a^*, a^*]^d\}} \\ = \sup_{f \in (\mathcal{F}_{a_0, M(a_0), W(a_0)}^{\mathbf{L}_d} \cap \mathcal{F}_{a^*, M(a^*)+1, W(a^*)+1}^{\mathbf{L}_d}) \setminus B_\epsilon(f_0)} \mathbb{E}[\{Y f(\mathbf{X}) - B(f(\mathbf{X}))\} \mathbb{1}_{\{\mathbf{X} \in [-a^*, a^*]^d\}}] \\ \leq \mathbb{E}[\{Y f_0(\mathbf{X}) - B(f_0(\mathbf{X}))\} \mathbb{1}_{\{\mathbf{X} \in [-a^*, a^*]^d\}}] - \zeta(a^*) \end{aligned} \quad (9)$$

$$\leq \bar{L}_0 - 2\zeta(a^*)/3, \quad (10)$$

where (9) is due to (6), and where (10) is due to (7). In addition, under the Binomial setting, for every $n \in \mathbb{N}$,

$$\sup_{f \in \mathcal{F}^{\mathbf{L}_d}} \frac{1}{n} \sum_{i=1}^n \{Y_i f(\mathbf{X}_i) - B(f(\mathbf{X}_i))\} \mathbb{1}_{\{\mathbf{X}_i \notin [-a^*, a^*]^d\}} \leq \frac{1}{n} \sum_{i=1}^n \sup_{t \in \mathbb{R}} \{Y_i t - B(t)\} \mathbb{1}_{\{\mathbf{X}_i \notin [-a^*, a^*]^d\}} \leq 0. \quad (11)$$

We deduce from (8), (10) and (11) that with probability one, $\hat{S}_n^{\mathbf{L}_d} \subseteq \text{cl}(B_\epsilon(f_0))$ for sufficiently large n . Finally, since $\text{cl}(B_\epsilon(f_0))|_{[-a_0, a_0]^d} = B_\epsilon(f_0)|_{[-a_0, a_0]^d}$, the conclusion of Theorem 2 for Binomial models follows.

Consistency of other EF additive models. The proof for other EF models follows the same structure, but involves some changes in certain places. We list the modifications required for each step here:

- In Step 1, we add a term independent of f to the definition of the partial log-likelihood:

$$\tilde{\ell}_n(f) = \frac{1}{n} \sum_{i=1}^n \left[Y_i f(\mathbf{X}_i) - B(f(\mathbf{X}_i)) - \sup_{t \in \text{dom}(B)} \{Y_i t - B(t)\} \right].$$

Note that

$$\sup_{t \in \text{dom}(B)} \{Y_i t - B(t)\} = \begin{cases} Y_i^2/2 & \text{if EF is Gaussian;} \\ Y_i \log Y_i - Y_i & \text{if EF is Poisson;} \\ -1 - \log Y_i & \text{if EF is Gamma.} \end{cases}$$

This allows us to prove that $\mathbb{E}\{\tilde{\ell}_n(f_0)\} \in (-\infty, 0]$ in all cases: in particular, in the Gaussian case, $\mathbb{E}\{\tilde{\ell}_n(f_0)\} = -\phi_0/4$; for the Poisson, we can use Lemma 13 in the online supplementary

material to see that $\mathbb{E}\{\tilde{\ell}_n(f_0)\} \in [-1, 0]$; for the Gamma, this claim follows from Lemma 14 in the online supplementary material. It then follows from the strong law of large numbers that almost surely

$$\liminf_{n \rightarrow \infty} \sup_{f \in \text{cl}(\mathcal{F}^{\mathbf{L}_d})} \tilde{\ell}_n(f) \geq \mathbb{E}\{\tilde{\ell}_n(f_0)\} =: \tilde{L}_0.$$

- In Step 2, the deterministic constant $M = M(a) \in (0, \infty)$ needs to be chosen differently for different EF distributions. Let $\mathcal{C}_a = \{C_1, \dots, C_N\}$ be the same finite collection of compact subsets defined previously. We then can pick

$$M = \begin{cases} 4 \left(\sqrt{\frac{2(-\tilde{L}_0+1)}{\min_{1 \leq k \leq N} \mathbb{P}(\mathbf{X} \in C_k, |Y| \leq 1)}} + 1 \right) & \text{if EF is Gaussian;} \\ 4 \left(\frac{-\tilde{L}_0+1}{\min_{1 \leq k \leq N} \mathbb{P}(\mathbf{X} \in C_k, Y=1)} + 1 \right) & \text{if EF is Poisson;} \\ 4 \left(\frac{2(-\tilde{L}_0+1)}{\min_{1 \leq k \leq N} \mathbb{P}(\mathbf{X} \in C_k, 1 \leq Y \leq e)} + 4 \right) & \text{if EF is Gamma.} \end{cases}$$

- Step 3 are exactly the same for all the EF distributions listed in Table 2.
- In Step 4, we define the class of functions

$$\begin{aligned} \tilde{\mathcal{H}}_{a, M_1, M_2} = & \left\{ h_f : \mathbb{R}^d \times \mathbb{R} \rightarrow \mathbb{R} \mid \right. \\ & \left. h_f(\mathbf{x}, y) = \left[yf(\mathbf{x}) - B(f(\mathbf{x})) - \sup_{t \in \text{dom}(B)} \{yt - B(t)\} \right] \mathbb{1}_{\{\mathbf{x} \in [-a, a]^d\}}, f \in \mathcal{F}_{a, M_1, M_2}^{\mathbf{L}_d} \right\}. \end{aligned}$$

In the Gaussian case, we can rewrite $h_f(\mathbf{x}, y) = -\frac{1}{2}\{y - f(\mathbf{x})\}^2 \mathbb{1}_{\{\mathbf{x} \in [-a, a]^d\}}$. By taking the P -integrable envelope function to be

$$F(\mathbf{x}, y) = \frac{1}{2}\{|y| + M_1(d+1)\}^2 \mathbb{1}_{\{\mathbf{x} \in [-a, a]^d\}} \geq \sup_{f \in \mathcal{F}_{a, M_1, M_2}^{\mathbf{L}_d}} |h_f(\mathbf{x}, y)|,$$

we can again deduce from Theorem 3 of van der Vaart and Wellner (2000) that $\tilde{\mathcal{H}}_{a, M_1, M_2}$ is P -Glivenko–Cantelli. Similarly, in the Poisson case, we can show that $\tilde{\mathcal{H}}_{a, M_1, M_2}$ is P -Glivenko–Cantelli by taking the envelope function to be $F(\mathbf{x}, y) = \{yM_1(d+1) + e^{M_1(d+1)} + y + y \log y\} \mathbb{1}_{\{\mathbf{x} \in [-a, a]^d\}}$.

The Gamma case is slightly more complex, mainly due to the fact that $\text{dom}(B) \neq \mathbb{R}$. For $\delta > 0$, let

$$\begin{aligned} \tilde{\mathcal{H}}_{a, M_1, M_2}^\delta = & \left\{ h_f : \mathbb{R}^d \times \mathbb{R} \rightarrow \mathbb{R} \mid \right. \\ & \left. h_f(\mathbf{x}, y) = \{yf(\mathbf{x}) + \log(\max(-f(\mathbf{x}), \delta)) - 1 + \log y\} \mathbb{1}_{\{\mathbf{x} \in [-a, a]^d\}}, f \in \mathcal{F}_{a, M_1, M_2}^{\mathbf{L}_d} \right\}. \end{aligned}$$

Again, we can show that $\tilde{\mathcal{H}}_{a, M_1, M_2}^\delta$ is P -Glivenko–Cantelli by taking the envelope function for $\tilde{\mathcal{H}}_{a, M_1, M_2}^\delta$ to be $F(\mathbf{x}, y) = \{yM_1(d+1) + |\log \delta| + |\log(M_1(d+1))| + 1 + \log y\} \mathbb{1}_{\{\mathbf{x} \in [-a, a]^d\}}$.

- Step 5 for the Gaussian and Poisson settings are essentially a replication of that for the Binomial case. Only very minor changes are required:

- (a) where applicable, add the term $-\sup_{t \in \mathbb{R}} [Yt - B(t)]$ to $\{Yf_0(\mathbf{X}) - B(f_0(\mathbf{X}))\}$ and $\{Yf(\mathbf{X}) - B(f(\mathbf{X}))\}$; make the respective change to $\{Y_i f(\mathbf{X}_i) - B(f(\mathbf{X}_i))\}$ and $\{yf(\mathbf{x}) - B(f(\mathbf{x}))\}$;
- (b) change \tilde{L}_0 to \tilde{L}_0 ;
- (c) change $\mathcal{H}_{a^*, M(a^*)+1, W(a^*)+1}$ to $\tilde{\mathcal{H}}_{a^*, M(a^*)+1, W(a^*)+1}$;
- (d) rewrite (11) as

$$\sup_{f \in \mathcal{F}^{\mathbf{L}_d}} \frac{1}{n} \sum_{i=1}^n \left[Y_i f(\mathbf{X}_i) - B(f(\mathbf{X}_i)) - \sup_{t \in \mathbb{R}} \{Y_i t - B(t)\} \right] \mathbb{1}_{\{\mathbf{X}_i \notin [-a^*, a^*]^d\}} \leq 0.$$

The analogue of Step 5 for the Gamma distribution is a little more involved. Set $\delta_0 = \inf_{\mathbf{x} \in [-a_0-1, a_0+1]^d} -f_0(\mathbf{x})/e^2 > 0$. Note that the above supremum is attained as f_0 is a continuous function. Then one can prove in a similar fashion to Lemma 11 that

$$\begin{aligned} \zeta &= \mathbb{E}[\{Yf_0(\mathbf{X}) + \log(-f_0(\mathbf{X})) + 1 + \log Y\} \mathbb{1}_{\{\mathbf{X} \in [-a_0-1, a_0+1]^d\}}] \\ &\quad - \sup_{f \in \mathcal{F}_{a_0, M(a_0), W(a_0)}^{\mathbf{L}_d} \setminus B_\epsilon(f_0)} \mathbb{E}[\{Yf(\mathbf{X}) + \log(\max(-f(\mathbf{X}), \delta_0)) + 1 + \log Y\} \mathbb{1}_{\{\mathbf{X} \in [-a_0-1, a_0+1]^d\}}] > 0. \end{aligned}$$

Next we pick $a^* > a_0 + 1$ such that

$$|\mathbb{E}[\{Yf_0(\mathbf{X}) + \log(-f_0(\mathbf{X})) + 1 + \log Y\} \mathbb{1}_{\{\mathbf{X} \notin [-a^*, a^*]^d\}}]| \leq \zeta/3$$

and $\delta^* = \inf_{\mathbf{x} \in [-a^*-1, a^*+1]^d} -f_0(\mathbf{x})/e^2$. Write

$$\mathcal{F}^{**} = \left(\mathcal{F}_{a_0, M(a_0), W(a_0)}^{\mathbf{L}_d} \cap \mathcal{F}_{a^*, M(a^*)+1, W(a^*)+1}^{\mathbf{L}_d} \right) \setminus B_\epsilon(f_0).$$

With \mathcal{F}^* defined as in Step 5, we have

$$\begin{aligned} &\left\{ \sup_{f \in \mathcal{F}^*} \frac{1}{n} \sum_{i=1}^n \{Y_i f(\mathbf{X}_i) + \log(-f(\mathbf{X}_i)) + 1 + \log Y_i\} \geq \tilde{L}_0 - \zeta/3 \right\} \\ &\subseteq \left\{ \sup_{f \in \mathcal{F}^{**}} \frac{1}{n} \sum_{i=1}^n \{Y_i f(\mathbf{X}_i) + \log(\max(-f(\mathbf{X}_i), \delta_0)) + 1 + \log Y_i\} \mathbb{1}_{\{\mathbf{X}_i \in [-a_0-1, a_0+1]^d\}} \right. \\ &\quad + \sup_{f \in \mathcal{F}^{**}} \frac{1}{n} \sum_{i=1}^n \{Y_i f(\mathbf{X}_i) + \log(\max(-f(\mathbf{X}_i), \delta^*)) + 1 + \log Y_i\} \mathbb{1}_{\{\mathbf{X}_i \in [-a^*, a^*]^d \setminus [-a_0-1, a_0+1]^d\}} \\ &\quad \left. + \sup_{f \in \mathcal{F}^{\mathbf{L}_d}} \frac{1}{n} \sum_{i=1}^n \{Y_i f(\mathbf{X}_i) + \log(-f(\mathbf{X}_i)) + 1 + \log Y_i\} \mathbb{1}_{\{\mathbf{X}_i \notin [-a^*, a^*]^d\}} \geq \tilde{L}_0 - \zeta/3 \right\}. \end{aligned}$$

Again we apply Glivenko–Cantelli theorem to finish the proof, where we also use the fact that

$$\begin{aligned} & \sup_{f \in \mathcal{F}^{**}} \mathbb{E} \left[\left\{ Y f(\mathbf{X}) + \log(\max(-f(\mathbf{X}), \delta^*)) + 1 + \log Y \right\} \mathbb{1}_{\{\mathbf{X} \in [-a^*, a^*]^d \setminus [-a_0-1, a_0+1]^d\}} \right] \\ & \leq \mathbb{E} \left[\left\{ Y f_0(\mathbf{X}) + \log(-f_0(\mathbf{X})) + 1 + \log Y \right\} \mathbb{1}_{\{\mathbf{X} \in [-a^*, a^*]^d \setminus [-a_0-1, a_0+1]^d\}} \right]. \end{aligned}$$

PROOF OF COROLLARY 3

By Theorem 2, we have

$$\sup_{\hat{f}_n \in \hat{S}_n^{\mathbf{L}^d}} |\hat{c}_n - c_0| = \sup_{\hat{f}_n \in \hat{S}_n^{\mathbf{L}^d}} |\hat{f}_n(\mathbf{0}) - f_0(\mathbf{0})| \xrightarrow{a.s.} 0$$

as $n \rightarrow \infty$. Moreover, writing $I_j = \{0\} \times \dots \times \{0\} \times [-a_0, a_0] \times \{0\} \times \dots \times \{0\}$, we have

$$\sup_{\hat{f}_n \in \hat{S}_n^{\mathbf{L}^d}} \sum_{j=1}^d \sup_{x_j \in [-a_0, a_0]} |\hat{f}_{n,j}(x_j) - f_{0,j}(x_j)| = \sup_{\hat{f}_n \in \hat{S}_n^{\mathbf{L}^d}} \sum_{j=1}^d \sup_{\mathbf{x} \in I_j} |\hat{f}_n(\mathbf{x}) - f_0(\mathbf{x}) - \hat{c}_n + c_0| \xrightarrow{a.s.} 0,$$

using Theorem 2 again and the triangle inequality.

PROOF OF PROPOSITION 4

Fix an index matrix $\mathbf{A} = (\boldsymbol{\alpha}_1, \dots, \boldsymbol{\alpha}_m) \in \mathbb{R}^{d \times m}$. For any sequence $\mathbf{A}^1, \mathbf{A}^2, \dots \in \mathbb{R}^{d \times m}$ with $\lim_{k \rightarrow \infty} \|\mathbf{A}^k - \mathbf{A}\|_F = 0$, where $\|\cdot\|_F$ denotes the Frobenius norm, we claim that $\lim_{k \rightarrow \infty} \|(\mathbf{A}^k)^T \mathbf{X}_i - \mathbf{A}^T \mathbf{X}_i\|_1 = 0$ for every $i = 1, \dots, n$. To see this, we write $\mathbf{A}^k = (\boldsymbol{\alpha}_1^k, \dots, \boldsymbol{\alpha}_m^k)$. It then follows that

$$\begin{aligned} \|(\mathbf{A}^k)^T \mathbf{X}_i - \mathbf{A}^T \mathbf{X}_i\|_1 &= \sum_{h=1}^m \left| ((\mathbf{A}^k)^T \mathbf{X}_i)_h - (\mathbf{A}^T \mathbf{X}_i)_h \right| = \sum_{h=1}^m \left| \sum_{j=1}^d (A_{jh}^k - A_{jh}) X_{ij} \right| \\ &\leq \sum_{h=1}^m \left[\|\mathbf{X}_i\|_2 \left\{ \sum_{j=1}^d (A_{jh}^k - A_{jh})^2 \right\}^{1/2} \right] \leq \|\mathbf{X}_i\|_2 \sqrt{m} \|\mathbf{A}^k - \mathbf{A}\|_F \rightarrow 0 \end{aligned}$$

as $k \rightarrow \infty$, where we have applied the Cauchy–Schwarz inequality twice. Now write $\mathbf{Z}_i = (Z_{i1}, \dots, Z_{im})^T = \mathbf{A}^T \mathbf{X}_i$ for every $i = 1, \dots, n$ and take

$$a^* = \max_{1 \leq i \leq n, 1 \leq j \leq m} |Z_{ij}|.$$

Since $\bigcup_{M=1}^{\infty} \mathcal{F}_{a^*, M}^{\mathbf{L}^m} = \mathcal{F}^{\mathbf{L}^m}$ (where $\mathcal{F}_{a^*, M}^{\mathbf{L}^m}$ is defined in (3)), it follows that

$$\lim_{M \rightarrow \infty} \sup_{f \in \mathcal{F}_{a^*, M}^{\mathbf{L}^m}} \bar{\ell}_{n,m}(f; (\mathbf{Z}_1, Y_1), \dots, (\mathbf{Z}_n, Y_n)) = \sup_{f \in \mathcal{F}^{\mathbf{L}^m}} \bar{\ell}_{n,m}(f; (\mathbf{Z}_1, Y_1), \dots, (\mathbf{Z}_n, Y_n)) = \Lambda_n(\mathbf{A}).$$

Therefore, for any $\epsilon > 0$, there exist $M_\epsilon > 0$ and $f^* \stackrel{\mathcal{F}^{\mathbf{L}^m}}{\sim} (f_1^*, \dots, f_m^*, c^*) \in \mathcal{F}_{a^*, M_\epsilon}^{\mathbf{L}^m}$ such that

$$\bar{\ell}_{n,m}(f^*; (\mathbf{Z}_1, Y_1), \dots, (\mathbf{Z}_n, Y_n)) \geq \Lambda_n(\mathbf{A}) - \epsilon.$$

We can then find piecewise linear and continuous functions $f_1^{**}, \dots, f_m^{**}$ such that $f_j^{**}(Z_{ij}) = f_j^*(Z_{ij})$ for every $i = 1, \dots, n, j = 1, \dots, m$. Consequently, the additive function $f^{**}(\mathbf{z}) = \sum_{j=1}^m f_j^{**}(z_j) + c^*$ is continuous. It now follows that

$$\begin{aligned} \liminf_{k \rightarrow \infty} \Lambda_n(\mathbf{A}^k) &\geq \liminf_{k \rightarrow \infty} \bar{\ell}_{n,m}(f^{**}; ((\mathbf{A}^k)^T \mathbf{X}_1, Y_1), \dots, ((\mathbf{A}^k)^T \mathbf{X}_n, Y_n)) \\ &= \bar{\ell}_{n,m}(f^{**}; (\mathbf{Z}_1, Y_1), \dots, (\mathbf{Z}_n, Y_n)) \\ &= \bar{\ell}_{n,m}(f^*; (\mathbf{Z}_1, Y_1), \dots, (\mathbf{Z}_n, Y_n)) \geq \Lambda_n(\mathbf{A}) - \epsilon. \end{aligned}$$

Since both $\epsilon > 0$ and the sequence (\mathbf{A}^k) were arbitrary, the result follows.

PROOF OF THEOREM 5

The structure of the proof is essentially the same as that of Theorem 2. For the sake of brevity, we focus on the main changes and on the Gaussian setting. Following the strategy used in the proof of Theorem 2, we work here with the logarithm of a normalised likelihood:

$$\begin{aligned} \tilde{\ell}_{n,m}(f; \mathbf{A}) &\equiv \tilde{\ell}_{n,m}(f; (\mathbf{A}^T \mathbf{X}_1, Y_1), \dots, (\mathbf{A}^T \mathbf{X}_n, Y_n)) \\ &= \bar{\ell}_{n,m}(f; (\mathbf{A}^T \mathbf{X}_1, Y_1), \dots, (\mathbf{A}^T \mathbf{X}_n, Y_n)) - \frac{1}{n} \sum_{i=1}^n \sup_{t \in \text{dom}(B)} \{Y_i t - B(t)\} \\ &= -\frac{1}{2n} \sum_{i=1}^n \{f(\mathbf{A}^T \mathbf{X}_i) - Y_i\}^2. \end{aligned}$$

So in Step 1, we can establish that $\mathbb{E} \tilde{\ell}_{n,m}(f_0; \mathbf{A}_0) = -\phi_0/4$.

In Step 2, we aim to bound \tilde{f}_n^I on $[-a, a]^d$ for any fixed $a > 0$. Three cases are considered:

- (a) If $m \geq 2$ and $\mathbf{L}_m \in \mathcal{L}_m$, then \tilde{f}_n^I is either convex or concave. One can now use the convexity/concavity to show that $\limsup_{n \rightarrow \infty} \sup_{\mathbf{x} \in [-a, a]^d} |\tilde{f}_n^I(\mathbf{x})| < M(a)$ almost surely for some deterministic constant $M(a) < \infty$ that only depends on a . See, for instance, Proposition 4 of Lim and Glynn (2012) for a similar argument.
- (b) Otherwise, if $\mathbf{L}_m \notin \mathcal{L}_m$, we will show that there exists deterministic $M(a) \in (0, \infty)$ such that with probability one,

$$\tilde{S}_n^{\mathbf{L}_m} \subseteq \mathcal{G}_{a, M(a)}^{\mathbf{L}_m, \delta} \tag{12}$$

for sufficiently large n , where we define

$$\mathcal{G}_{a, M}^{\mathbf{L}_m, \delta} = \left\{ f^I : \mathbb{R}^d \rightarrow \mathbb{R} \mid f^I(\mathbf{x}) = f(\mathbf{A}^T \mathbf{x}), \text{ with } f \in \mathcal{F}_{a, M}^{\mathbf{L}_m} \text{ and } \mathbf{A} \in \mathcal{A}_d^{\mathbf{L}_m, \delta} \right\}.$$

To see this, we first extend Lemma 7 to the following:

Lemma 8. Fix $a > 0$ and $\delta > 0$, and set $\tilde{\delta} = \min(\delta, d^{-1})$. For every $f^I(\mathbf{x}) = f(\mathbf{A}^T \mathbf{x}) = \sum_{j=1}^m f_j(\boldsymbol{\alpha}_j^T \mathbf{x}) + c$ with $f \stackrel{\mathcal{F}^{\mathbf{L}^m}}{\sim} (f_1, \dots, f_m, c)$ and $\mathbf{A} \in \mathcal{A}_d^{\mathbf{L}^m, \delta}$, there exists a convex, compact subset D_{f^I} of $[-2\tilde{\delta}^{-1/2}ad, 2\tilde{\delta}^{-1/2}ad]^d$ having Lebesgue measure $(\frac{a}{2d})^d$ such that

$$\max \left\{ \inf_{\mathbf{x} \in D_{f^I}} f^I(\mathbf{x}), \inf_{\mathbf{x} \in D_{f^I}} -f^I(\mathbf{x}) \right\} \geq \frac{1}{4} \max \left\{ \sup_{|z_1| \leq a} |f_1(z_1)|, \dots, \sup_{|z_m| \leq a} |f_m(z_m)|, 2|c| \right\}. \quad (13)$$

Proof. First consider the case $m = d$. Note that every $\mathbf{A} \in \mathcal{A}_d^{\mathbf{L}^d, \delta}$ is invertible. In fact, if λ is an eigenvalue of \mathbf{A} , then $\delta^{1/2} \leq |\lambda| \leq 1$, where the upper bound follows from the Gerschgorin circle theorem (Gerschgorin, 1931; Gradshteyn and Ryzhik, 2007). Let C_1, \dots, C_N be the sets constructed for f in Lemma 7. Then, writing ν_d for Lebesgue measure on \mathbb{R}^d ,

$$\min_{1 \leq k \leq N} \nu_d((\mathbf{A}^T)^{-1} C_k) \geq \frac{1}{|\det(\mathbf{A}^T)|} \min_{1 \leq k \leq N} \nu_d(C_k) \geq \left(\frac{a}{2d} \right)^d,$$

and

$$\bigcup_{1 \leq k \leq N} (\mathbf{A}^T)^{-1} C_k \subseteq (\mathbf{A}^T)^{-1} [-2a, 2a]^d \subseteq [-2\tilde{\delta}^{-1/2}ad, 2\tilde{\delta}^{-1/2}ad]^d.$$

Thus (13) is satisfied. To complete the proof of this lemma, we note that for any $m < d$, we can always find a $d \times (d - m)$ matrix $\mathbf{B} = (\boldsymbol{\beta}_1, \dots, \boldsymbol{\beta}_{d-m})$ such that

1. $\|\boldsymbol{\beta}_j\|_1 = 1$ for every $j = 1, \dots, d - m$.
2. $\boldsymbol{\beta}_j^T \boldsymbol{\beta}_k = 0$ for every $1 \leq j < k \leq d - m$.
3. $\mathbf{A}^T \mathbf{B} = 0$.

Let $\mathbf{A}_+ = (\mathbf{A}, \mathbf{B})$, so the modulus of every eigenvalue of \mathbf{A}_+ belongs to $[\min(\delta^{1/2}, d^{-1/2}), 1]$. Since $f^I(\mathbf{x}) = f(\mathbf{A}^T \mathbf{x}) \equiv f'(\mathbf{A}_+^T \mathbf{x})$ with $f'(\mathbf{z}) = \sum_{j=1}^m f_j(z_j) + c$ for every $\mathbf{z} = (z_1, \dots, z_d)^T \in \mathbb{R}^d$, the problem reduces to the case $m = d$. \square

Then, instead of using the strong law of large numbers to complete this step, we apply the Glivenko–Cantelli theorem for classes of convex sets (Bhattacharya and Rao, 1976, Theorem 1.11). This change is necessary to circumvent the fact that the set D_{f^I} depends on the function f^I (via its index matrix \mathbf{A}).

- (c) Finally, if $m = 1$, then the Cauchy–Schwarz inequality gives that $\mathcal{A}_d^{L_1} \equiv \mathcal{A}_d^{L_1, \delta}$ with $\delta = d^{-1}$. Thus (12) still holds true.

Two different cases are considered in Step 4:

- (a) If $m \geq 2$ and $\mathbf{L}_m \in \mathcal{L}_m$, then without loss of generality, we can assume $\mathbf{L}_m \in \{1, 4, 5, 6\}^m$. It is enough to show that the set of functions

$$\mathcal{G}_{a, M_1, M_2}^{\mathbf{L}_m, d} = \left\{ h_f : \mathbb{R}^d \times \mathbb{R} \rightarrow \mathbb{R} \mid h_f(\mathbf{x}, y) = -\frac{1}{2} \{f(\mathbf{x}) - y\}^2 \mathbb{1}_{\{\mathbf{x} \in [-a, a]^d\}} \text{ with } f : \mathbb{R}^d \rightarrow \mathbb{R} \text{ convex,} \right. \\ \left. \sup_{\mathbf{x} \in [-a, a]^d} |f(\mathbf{x})| \leq M_1 \text{ and } |f(\mathbf{x}_1) - f(\mathbf{x}_2)| \leq M_2 \|\mathbf{x}_1 - \mathbf{x}_2\| \text{ for any } \mathbf{x}_1, \mathbf{x}_2 \in [-a, a]^d \right\}$$

is P -Glivenko–Cantelli, where P is the distribution of (\mathbf{X}, Y) . This follows from an application of Corollary 2.7.10 and Theorem 2.4.1 of van der Vaart and Wellner (1996), as well as Theorem 3 of van der Vaart and Wellner (2000).

- (b) Otherwise, we need to show that the set of functions

$$\mathcal{G}_{a, M_1, M_2}^{\mathbf{L}_m, d, \delta} = \left\{ h_{f, \mathbf{A}} : \mathbb{R}^d \times \mathbb{R} \rightarrow \mathbb{R} \mid h_{f, \mathbf{A}}(\mathbf{x}, y) = -\frac{1}{2} \{f(\mathbf{A}^T \mathbf{x}) - y\}^2 \mathbb{1}_{\{\mathbf{x} \in [-a, a]^d\}} \right. \\ \left. \text{with } f \in \mathcal{F}_{a, M_1, M_2}^{\mathbf{L}_m} \text{ and } \mathbf{A} \in \mathcal{A}_d^{\mathbf{L}_m, \delta} \right\}$$

is P -Glivenko–Cantelli. The proof is similar to that given in Step 4 of the proof of Theorem 2. The compactness of $\mathcal{A}_d^{\mathbf{L}_m, \delta}$, together with a bracketing number argument is used here to establish the claim. See Lemma 15 in the online supplementary material for details.

PROOF OF COROLLARY 6

This result follows from Theorem 1 of Yuan (2011) and our Theorem 5. See also Theorem 5 of Samworth and Yuan (2012) for a similar type of argument.

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ONLINE SUPPLEMENTARY MATERIAL

Recall the definition of Θ from the proof of Proposition 1.

Lemma 9. *The set Θ is a closed subset of $\bar{\mathbb{R}}^n$.*

Proof. Suppose that, for each $m \in \mathbb{N}$, the vector $\boldsymbol{\eta}^m = (\eta_1^m, \dots, \eta_n^m)^T$ belongs to Θ , and that $\boldsymbol{\eta}^m \rightarrow \boldsymbol{\eta} = (\eta_1, \dots, \eta_n)^T$ as $m \rightarrow \infty$. Then, for each $m \in \mathbb{N}$, there exists a sequence $(f^{m,k}) \in \mathcal{F}^{\mathbf{L}_d}$ such that $f^{m,k}(\mathbf{X}_i) \rightarrow \eta_i^m$ as $k \rightarrow \infty$ for $i = 1, \dots, n$. It follows that we can find $k_m \in \mathbb{N}$ such that $f^{m,k_m}(\mathbf{X}_i) \rightarrow \eta_i$ as $m \rightarrow \infty$, for each $i = 1, \dots, n$.

For $j = 1, \dots, d$, let $\{X_{(i),j}\}_{i=1}^{N_j}$ denote the distinct order statistics of $\{X_{ij}\}_{i=1}^n$ (thus $N_j < n$ if there are ties among $\{X_{ij}\}_{i=1}^n$). Moreover, let

$$\mathcal{V}_j = \{(-\infty, X_{(1),j}], [X_{(1),j}, X_{(2),j}], \dots, [X_{(N_j-1),j}, X_{(N_j),j}], [X_{(N_j),j}, \infty)\},$$

and let $\mathcal{V} = \times_{j=1}^d \mathcal{V}_j$. Thus $|\mathcal{V}| = \prod_{j=1}^d (N_j + 1)$ and the union of all the sets in \mathcal{V} is \mathbb{R}^d . Writing $f^{m,k_m} \stackrel{\mathcal{F}^{\mathbf{L}_d}}{\sim} (f_1^{m,k_m}, \dots, f_d^{m,k_m}, c^{m,k_m})$, we define a modified sequence $\tilde{f}^m \stackrel{\mathcal{F}^{\mathbf{L}_d}}{\sim} (\tilde{f}_1^m, \dots, \tilde{f}_d^m, \tilde{c}^m)$ at $\mathbf{x} = (x_1, \dots, x_d)^T \in \mathbb{R}^d$ by setting

$$\tilde{f}_j^m(x_j) = \begin{cases} \frac{(X_{(i+1),j} - x_j)f_j^{m,k_m}(X_{(i),j})}{X_{(i+1),j} - X_{(i),j}} + \frac{(x_j - X_{(i),j})f_j^{m,k_m}(X_{(i+1),j})}{X_{(i+1),j} - X_{(i),j}} & \text{if } x_j \in [X_{(i),j}, X_{(i+1),j}] \\ \frac{(X_{(2),j} - x_j)f_j^{m,k_m}(X_{(1),j})}{X_{(2),j} - X_{(1),j}} + \frac{(x_j - X_{(1),j})f_j^{m,k_m}(X_{(2),j})}{X_{(2),j} - X_{(1),j}} & \text{if } x_j \in (-\infty, X_{(1),j}] \\ \frac{(X_{(N_j),j} - x_j)f_j^{m,k_m}(X_{(N_j-1),j})}{X_{(N_j),j} - X_{(N_j-1),j}} + \frac{(x_j - X_{(N_j-1),j})f_j^{m,k_m}(X_{(N_j),j})}{X_{(N_j),j} - X_{(N_j-1),j}} & \text{if } x_j \in [X_{(N_j),j}, \infty), \end{cases}$$

and $\tilde{c}^m = c^{m,k_m}$. Thus each component function \tilde{f}_j^m is piecewise linear, continuous and satisfies the same shape constraint as f_j^{m,k_m} , and \tilde{f}^m is piecewise affine and $\tilde{f}^m(\mathbf{X}_i) = f^{m,k_m}(\mathbf{X}_i) = \eta_i^m$ for $i = 1, \dots, n$. The proof will therefore be concluded if we can show that a subsequence of (\tilde{f}^m) converges pointwise in $\bar{\mathbb{R}}$. To do this, it suffices to show that, given an arbitrary $V \in \mathcal{V}$, we can find a subsequence of $(\tilde{f}^m|_V)$ (where $\tilde{f}^m|_V$ denotes the restriction of \tilde{f}^m to V) converging pointwise in $\bar{\mathbb{R}}$. Note that we can write

$$\tilde{f}^m|_V(\mathbf{x}) = (\mathbf{a}^m)^T(\mathbf{x}^T, 1)^T$$

for some $\mathbf{a}^m = (a_1^m, \dots, a_{d+1}^m)^T \in \mathbb{R}^{d+1}$. If the sequence (\mathbf{a}^m) is bounded, then we can find a subsequence (\mathbf{a}^{m_k}) , converging to $\mathbf{a} \in \mathbb{R}^{d+1}$, say. In that case, for all $\mathbf{x} \in V$, we have $\tilde{f}^{m_k}|_V(\mathbf{x}) \rightarrow \mathbf{a}^T(\mathbf{x}^T, 1)^T$, and we are done. On the other hand, if (\mathbf{a}^m) is unbounded, we can let $j^m = \operatorname{argmax}_{j=1, \dots, d+1} |a_j^m|$, where we choose the largest index in the case of ties. Since j^m can only take $d+1$ values, we may assume without loss of generality that there is a subsequence (j^{m_k}) such that $j^{m_k} = d+1$ for all $k \in \mathbb{N}$ and such that $a_{d+1}^{m_k} \rightarrow \infty$ as $k \rightarrow \infty$. By choosing further

subsequences if necessary, we may also assume that

$$\left(\frac{a_1^{m_k}}{a_{d+1}^{m_k}}, \dots, \frac{a_d^{m_k}}{a_{d+1}^{m_k}} \right)^T \rightarrow (\tilde{a}_1, \dots, \tilde{a}_d)^T =: \tilde{\mathbf{a}},$$

say, where $\tilde{\mathbf{a}} \in [-1, 1]^d$. Writing $V_1 = \{\mathbf{x} \in V : (\tilde{\mathbf{a}}^T, 1)(\mathbf{x}^T, 1)^T = 0\}$, $V_1^+ = \{\mathbf{x} \in V : (\tilde{\mathbf{a}}^T, 1)(\mathbf{x}^T, 1)^T > 0\}$ and $V_1^- = \{\mathbf{x} \in V : (\tilde{\mathbf{a}}^T, 1)(\mathbf{x}^T, 1)^T < 0\}$, we deduce that for large k ,

$$\tilde{f}^{m_k}|_V(\mathbf{x}) = a_{d+1}^{m_k} \left(\frac{a_1^{m_k}}{a_{d+1}^{m_k}}, \dots, \frac{a_d^{m_k}}{a_{d+1}^{m_k}}, 1 \right)^T (\mathbf{x}^T, 1)^T \rightarrow \begin{cases} \infty & \text{if } \mathbf{x} \in V_1^+ \\ -\infty & \text{if } \mathbf{x} \in V_1^-. \end{cases}$$

It therefore suffices to consider $\tilde{f}^{m_k}|_{V_1}$. We may assume that $\tilde{\mathbf{a}} \neq \mathbf{0}$ (otherwise $V_1 = \emptyset$ and we are done), so without loss of generality assume $\tilde{a}_d \neq 0$. But then, for $\mathbf{x} \in V_1$,

$$\tilde{f}^{m_k}|_{V_1}(\mathbf{x}) = (\mathbf{a}^{m_k})^T (\mathbf{x}^T, 1)^T = (\mathbf{b}^{m_k})^T (\mathbf{x}_{(-d)}^T, 1)^T,$$

where $\mathbf{x}_{(-d)} = (x_1, \dots, x_{d-1})^T$, and where $\mathbf{b}^{m_k} = (b_1^{m_k}, \dots, b_d^{m_k}) \in \mathbb{R}^d$, with $b_j^{m_k} = a_j^{m_k} - \frac{a_d^{m_k}}{\tilde{a}_d} \tilde{a}_j$ for $j = 1, \dots, d-1$ and $b_d^{m_k} = a_{d+1}^{m_k} - \frac{a_d^{m_k}}{\tilde{a}_d}$. Applying the same argument inductively, we find subsets V_2, \dots, V_{d+1} , where $V_1 \supseteq V_2 \supseteq \dots \supseteq V_{d+1}$, where V_j has dimension $d-j$ and $V_{d+1} = \emptyset$, such that a subsequence of (\tilde{f}^{m_k}) converges pointwise in $\bar{\mathbb{R}}$ for all $\mathbf{x} \in V \setminus V_j$. \square

Now recall the definitions of $\mathcal{F}_{a,M}^{\mathbf{L}_d}$, $\mathcal{F}_{a,M_1,M_2}^{\mathbf{L}_d}$, $M(a)$ and $W(a)$ from the proof of Theorem 2.

Lemma 10. *For any $a > 0$, we have $\text{cl}(\mathcal{F}_{a,M(a)}^{\mathbf{L}_d}) \cap \text{cl}(\mathcal{F}_{a+1,M(a+1)}^{\mathbf{L}_d}) \subseteq \text{cl}(\mathcal{F}_{a,M(a),W(a)}^{\mathbf{L}_d})$.*

Proof. We first consider the case $M(a) \leq M(a+1)$. Suppose $f \in \text{cl}(\mathcal{F}_{a,M(a)}^{\mathbf{L}_d}) \cap \text{cl}(\mathcal{F}_{a+1,M(a+1)}^{\mathbf{L}_d})$, so there exists a sequence (f^k) such that $f^k \in \mathcal{F}_{a,M(a)}^{\mathbf{L}_d}$ and such that $f^k \xrightarrow{\mathcal{F}^{\mathbf{L}_d}} (f_1^k, \dots, f_d^k, c^k)$ converges pointwise in $\bar{\mathbb{R}}$ to f . Our first claim is that there exists a subsequence (f^{k_m}) such that $f^{k_m} \in \mathcal{F}_{a+1,M(a+1)+1}^{\mathbf{L}_d}$ for every $m \in \mathbb{N}$.

Indeed, suppose for a contradiction that there exists $K \in \mathbb{N}$ such that for every $k \geq K$, we have $f^k \notin \mathcal{F}_{a+1,M(a+1)+1}^{\mathbf{L}_d}$. Let

$$\mathbf{b}^k = (b_1^k, \dots, b_{2d+1}^k)^T = \left(|f_1^k(-a-1)|, |f_1^k(a+1)|, \dots, |f_d^k(-a-1)|, |f_d^k(a+1)|, 2|c^k| \right)^T.$$

It follows from our hypothesis and the shape restrictions that $\max_{j=1, \dots, 2d+1} b_j^k > M(a+1) + 1$ for $k \geq K$. Furthermore, we cannot have $\arg\max_{j=1, \dots, 2d+1} b_j^k = 2d+1$ for any $k \geq K$, because $2|c^k| = 2|f^k(\mathbf{0})| \leq M(a) < M(a+1) + 1$ for every $k \in \mathbb{N}$. We therefore let $j^k = \arg\max_{j=1, \dots, 2d} b_j^k$, where we choose the largest index in the case of ties. Since j^k can only take $2d$ values, we may

assume without loss of generality that there is a subsequence (j^{k_m}) such that $j^{k_m} = 2d$ for all $m \in \mathbb{N}$. But, writing $\mathbf{x}_0 = (0, \dots, 0, a+1)^T \in \mathbb{R}^d$, this implies that

$$|f(\mathbf{x}_0) - f(\mathbf{0})| = \lim_{m \rightarrow \infty} |f^{k_m}(\mathbf{x}_0) - f^{k_m}(\mathbf{0})| = \lim_{m \rightarrow \infty} |f_d^{k_m}(a+1)| \geq M(a+1) + 1.$$

On the other hand, since $f \in \text{cl}(\mathcal{F}_{a+1, M(a+1)}^{\mathbf{L}_d})$, we can find $(\tilde{f}^m) \in \mathcal{F}_{a+1, M(a+1)}^{\mathbf{L}_d}$ such that $\tilde{f}^m \xrightarrow{\mathcal{F}_d^{\mathbf{L}_d}} (f_1^m, \dots, f_d^m, \tilde{c}^m)$ converges pointwise in $\bar{\mathbb{R}}$ to f . So

$$|f(\mathbf{x}_0) - f(\mathbf{0})| = \lim_{m \rightarrow \infty} |\tilde{f}^m(\mathbf{x}_0) - \tilde{f}^m(\mathbf{0})| = \lim_{m \rightarrow \infty} |\tilde{f}_d^m(a+1)| \leq M(a+1).$$

This contradiction establishes our first claim. Since $\mathcal{F}_{a, M(a)}^{\mathbf{L}_d} \cap \mathcal{F}_{a+1, M(a+1)+1}^{\mathbf{L}_d} \subseteq \mathcal{F}_{a, M(a), W(a)}^{\mathbf{L}_d}$, we deduce that $f \in \text{cl}(\mathcal{F}_{a, M(a), W(a)}^{\mathbf{L}_d})$ in the case where $M(a) \leq M(a+1)$.

Now if $M(a) > M(a+1)$, then for every $f \in \text{cl}(\mathcal{F}_{a, M(a)}^{\mathbf{L}_d}) \cap \text{cl}(\mathcal{F}_{a+1, M(a+1)}^{\mathbf{L}_d})$, there exists a sequence (f^k) such that $f^k \in \mathcal{F}_{a+1, M(a+1)}^{\mathbf{L}_d}$ and such that f^k converges pointwise in $\bar{\mathbb{R}}$ to f . By the shape restrictions, $\mathcal{F}_{a+1, M(a+1)}^{\mathbf{L}_d} \subseteq \mathcal{F}_{a, M(a)}^{\mathbf{L}_d}$, so $f^k \in \mathcal{F}_{a, M(a)}^{\mathbf{L}_d}$. Consequently, $f^k \in \mathcal{F}_{a, M(a), W(a)}^{\mathbf{L}_d}$ as above, so $f \in \text{cl}(\mathcal{F}_{a, M(a), W(a)}^{\mathbf{L}_d})$. \square

Lemma 11. *Under assumptions (A.1) - (A.4), for any $a, M_1, M_2, \epsilon > 0$,*

$$\begin{aligned} & \mathbb{E}[\{Y f_0(\mathbf{X}) - B(f_0(\mathbf{X}))\} \mathbb{1}_{\{\mathbf{X} \in [-a-1, a+1]^d\}}] \\ & > \sup_{f \in \mathcal{F}_{a, M_1, M_2}^{\mathbf{L}_d} \setminus B_\epsilon(f_0)} \mathbb{E}[\{Y f(\mathbf{X}) - B(f(\mathbf{X}))\} \mathbb{1}_{\{\mathbf{X} \in [-a-1, a+1]^d\}}]. \end{aligned}$$

Proof. Since $B' = g^{-1}$, we have that for every $\mathbf{x} \in [-a-1, a+1]^d$, the expression

$$\mathbb{E}\{Y f(\mathbf{X}) - B(f(\mathbf{X})) | \mathbf{X} = \mathbf{x}\} = g^{-1}(f_0(\mathbf{x}))f(\mathbf{x}) - B(f(\mathbf{x}))$$

is uniquely maximised by taking $f(\mathbf{x}) = f_0(\mathbf{x})$. Moreover, since f_0 is continuous by assumption (A.4), it is uniformly continuous on $[-a-1, a+1]^d$. We may therefore assume that for any $\epsilon' > 0$, there exists $\gamma(\epsilon') > 0$ such that $|f_{0,j}(z_1) - f_{0,j}(z_2)| < \epsilon'$ for every $j = 1, \dots, d$ and every $z_1, z_2 \in [-a-1, a+1]$ with $|z_1 - z_2| < \gamma(\epsilon')$. For any $f \in \mathcal{F}_{a, M_1, M_2}^{\mathbf{L}_d} \setminus B_\epsilon(f_0)$, there exists $\mathbf{x}^* = (x_1^*, \dots, x_d^*)^T \in [-a, a]^d$ such that $|f(\mathbf{x}^*) - f_0(\mathbf{x}^*)| > \epsilon$. Let $C_{\mathbf{x}^*, 1} = \times_{j=1}^d D_j \subseteq [-a-1, a+1]^d$ where

$$D_j = \begin{cases} [x_j^*, x_j^* + \min\{\gamma(\frac{\epsilon}{2d}), 1\}] & \text{if } l_j = 2 \\ [x_j^* - \min\{\gamma(\frac{\epsilon}{2d}), 1\}, x_j^*] & \text{if } l_j = 3 \\ \left[x_j^* - \min\left\{\frac{1}{M_2} \frac{\epsilon}{4d}, \gamma(\frac{\epsilon}{4d}), 1\right\}, x_j^* + \min\left\{\frac{1}{M_2} \frac{\epsilon}{4d}, \gamma(\frac{\epsilon}{4d}), 1\right\} \right] & \text{if } l_j \in \{1, 4, 5, 6, 7, 8, 9\}. \end{cases}$$

Define $C_{\mathbf{x}^*,2}$ similarly, but with the intervals in the cases $l_j = 2$ and $l_j = 3$ exchanged. Then the shape constraints ensure that $\max\{\inf_{\mathbf{x} \in C_{\mathbf{x}^*,1}} |f(\mathbf{x}) - f_0(\mathbf{x})|, \inf_{\mathbf{x} \in C_{\mathbf{x}^*,2}} |f(\mathbf{x}) - f_0(\mathbf{x})|\} > \epsilon/2$. But the d -dimensional Lebesgue measures of $C_{\mathbf{x}^*,1}$ and $C_{\mathbf{x}^*,2}$ do not depend on \mathbf{x}^* , and $\min\{\mathbb{P}(\mathbf{X} \in C_{\mathbf{x}^*,1}), \mathbb{P}(\mathbf{X} \in C_{\mathbf{x}^*,2})\}$ is a continuous function of \mathbf{x}^* , so by (A.2), we have

$$\xi = \inf_{\mathbf{x}^* \in [-a,a]^d} \min\{\mathbb{P}(\mathbf{X} \in C_{\mathbf{x}^*,1}), \mathbb{P}(\mathbf{X} \in C_{\mathbf{x}^*,2})\} > 0.$$

Moreover, writing $\underline{f}_0 = \inf_{\mathbf{x} \in [-a-1,a+1]^d} f_0(\mathbf{x})$ and $\bar{f}_0 = \sup_{\mathbf{x} \in [-a-1,a+1]^d} f_0(\mathbf{x})$, and using the fact that $s \mapsto [\{g^{-1}(f_0(\mathbf{x}))f_0(\mathbf{x}) - B(f_0(\mathbf{x}))\} - \{g^{-1}(f_0(\mathbf{x}))s - B(s)\}]$ is convex, we deduce that

$$\begin{aligned} & \mathbb{E}[\{Y f_0(\mathbf{X}) - B(f_0(\mathbf{X}))\} \mathbb{1}_{\{\mathbf{X} \in [-a-1,a+1]^d\}}] \\ & - \sup_{f \in \mathcal{F}_{a,M_1,M_2}^{\mathbf{L}_d} \setminus B_\epsilon(f_0)} \mathbb{E}[\{Y f(\mathbf{X}) - B(f(\mathbf{X}))\} \mathbb{1}_{\{\mathbf{X} \in [-a-1,a+1]^d\}}] \\ & \geq \xi \inf_{\mathbf{x} \in [-a-1,a+1]^d} \inf_{|t-f_0(\mathbf{x})| > \epsilon/2} [\{g^{-1}(f_0(\mathbf{x}))f_0(\mathbf{x}) - B(f_0(\mathbf{x}))\} - \{g^{-1}(f_0(\mathbf{x}))t - B(t)\}] \\ & \geq \frac{1}{16} \xi \epsilon^2 \inf_{s \in [\underline{f}_0 - \epsilon/2, \bar{f}_0 + \epsilon/2]} (g^{-1})'(s) > 0. \end{aligned}$$

□

Lemma 12. *For any $a^* > a_0 + 1$, we have*

$$\begin{aligned} & \text{cl}\left(\mathcal{F}_{a_0,M(a_0)}^{\mathbf{L}_d} \setminus B_\epsilon(f_0)\right) \cap \text{cl}\left(\mathcal{F}_{a_0+1,M(a_0+1)}^{\mathbf{L}_d} \setminus B_\epsilon(f_0)\right) \cap \text{cl}\left(\mathcal{F}_{a^*,M(a^*)}^{\mathbf{L}_d} \setminus B_\epsilon(f_0)\right) \\ & \cap \text{cl}\left(\mathcal{F}_{a^*+1,M(a^*+1)}^{\mathbf{L}_d} \setminus B_\epsilon(f_0)\right) \subseteq \text{cl}\left(\left(\mathcal{F}_{a_0,M(a_0),W(a_0)}^{\mathbf{L}_d} \cap \mathcal{F}_{a^*,M(a^*)+1,W(a^*)+1}^{\mathbf{L}_d}\right) \setminus B_\epsilon(f_0)\right). \end{aligned}$$

Proof. The proof is very similar indeed to the proof of Lemma 10, so we omit the details. □

Recall the definition of $\tilde{l}_n(f_0)$ from the proof of Theorem 2.

Lemma 13. *Suppose that Z has a Poisson distribution with mean $\mu \in (0, \infty)$. Then*

$$\mu \log \mu \leq \mathbb{E}(Z \log Z) \leq \mu \log \mu + 1.$$

It follows that, under the Poisson setting, $\mathbb{E}\{\tilde{l}_n(f_0)\} \in [-1, 0]$.

Proof. The lower bound is immediate from Jensen's inequality. For the upper bound, let $Z_0 = (Z - \mu)/\sqrt{\mu}$, so $\mathbb{E}(Z_0) = 0$ and $\mathbb{E}(Z_0^2) = 1$. It follows from the inequality $\log(1+z) \leq z$ for any

$z > -1$ that

$$\begin{aligned}\mathbb{E}(Z \log Z) &= \mathbb{E}[(\mu + \sqrt{\mu}Z_0)\{\log \mu + \log(1 + Z_0/\sqrt{\mu})\}\mathbb{1}_{\{Z_0 > -\sqrt{\mu}\}}] \\ &\leq \mathbb{E}[(\mu + \sqrt{\mu}Z_0)(\log \mu + Z_0/\sqrt{\mu})] \\ &= \mu \log \mu + (\log \mu + 1)\sqrt{\mu}\mathbb{E}(Z_0) + \mathbb{E}(Z_0^2) = \mu \log \mu + 1.\end{aligned}$$

Finally, we note that

$$\begin{aligned}\mathbb{E}\tilde{l}_n(f_0) &= \mathbb{E}[\mathbb{E}\{Y f_0(\mathbf{X}) - B(f_0(\mathbf{X})) - Y \log Y + Y | \mathbf{X}\}] \\ &= \mathbb{E}\{e^{f_0(\mathbf{X})} f_0(\mathbf{X}) - \mathbb{E}(Y \log Y | \mathbf{X})\} \in [-1, 0].\end{aligned}$$

□

Lemma 14. *In the Gamma setting, under assumption (A.1) and (A.3), $\mathbb{E}\{\tilde{l}_n(f_0)\} \in (-\infty, 0)$.*

Proof. Since $-Y f_0(\mathbf{X}) | \mathbf{X} \sim \Gamma(1/\phi_0, 1/\phi_0)$, we have

$$\begin{aligned}\mathbb{E}\tilde{l}_n(f_0) &= \mathbb{E}[\mathbb{E}\{Y f_0(\mathbf{X}) - B(f_0(\mathbf{X})) - \log Y + 1 | \mathbf{X}\}] = \mathbb{E}[\mathbb{E}\{\log(-Y f_0(\mathbf{X})) | \mathbf{X}\}] \\ &= \log \phi_0 + \psi_D(1/\phi_0) \in (-\infty, 0),\end{aligned}$$

where $\psi_D(\cdot)$ denotes the digamma function. □

Lemma 15. *In the Gaussian setting, under (A.1)-(A.2) and (B.2)-(B.3),*

$$\begin{aligned}\mathcal{G}_{a, M_1, M_2}^{\mathbf{L}_m, d, \delta} &= \left\{ h_{f, \mathbf{A}} : \mathbb{R}^d \times \mathbb{R} \rightarrow \mathbb{R} \mid h_{f, \mathbf{A}}(\mathbf{x}, y) = -\frac{1}{2} \{f(\mathbf{A}^T \mathbf{x}) - y\}^2 \mathbb{1}_{\{\mathbf{x} \in [-a, a]^d\}} \right. \\ &\quad \left. \text{with } f \in \mathcal{F}_{a, M_1, M_2}^{\mathbf{L}_m} \text{ and } \mathbf{A} \in \mathcal{A}_{d, \delta}^{\mathbf{L}_m} \right\}\end{aligned}$$

is P -Glivenko–Cantelli.

Proof. Following the argument in Step 4 of the proof of Theorem 2, it suffices to show that

$$\begin{aligned}(\mathring{\mathcal{F}}_{a, M_1, M_2}^{\mathbf{L}_d})_j &= \left\{ \mathring{f} : \mathbb{R}^d \rightarrow \mathbb{R} \mid \mathring{f}(\mathbf{x}) = f_j(\boldsymbol{\alpha}_j^T \mathbf{x}) \mathbb{1}_{\{\mathbf{x} \in [-a, a]^d\}} \text{ for some } f \stackrel{\mathcal{F}^{\mathbf{L}_d}}{\sim} (f_1, \dots, f_m, c) \in \mathcal{F}_{a, M_1, M_2}^{\mathbf{L}_m} \right. \\ &\quad \left. \text{and } \boldsymbol{\alpha}_j \in \mathbb{R}^d \text{ with } \|\boldsymbol{\alpha}_j\|_1 = 1 \right\}\end{aligned}$$

is P -Glivenko–Cantelli for every $j = 1, \dots, m$. In the following, we present the proof in case $l_j = 2$. Other cases can be shown in a similar manner.

By Theorem 2.7.5 of van der Vaart and Wellner (1996), there exists a universal constant $C > 0$ such that for any $\epsilon > 0$ and any $\boldsymbol{\alpha}_0 \in \mathbb{R}^d$, there exist functions $g_k^L, g_k^U : \mathbb{R} \rightarrow [0, 1]$ for $k = 1, \dots, N_3$

with $N_3 = e^{4M_1C/\epsilon}$ such that $\mathbb{E}|g_k^U(\alpha_0^T \mathbf{X}) - g_k^L(\alpha_0^T \mathbf{X})| \leq \epsilon/(4M_1)$ and such that for every monotone function $g : \mathbb{R} \rightarrow [0, 1]$, we can find $k^* \in \{1, \dots, N_3\}$ with $g_{k^*}^L \leq g \leq g_{k^*}^U$. Since \mathbf{X} has a Lebesgue density, for every k we can find $\tau_k^L, \tau_k^U > 0$ such that

$$\mathbb{E}|g_k^L(\alpha_0^T \mathbf{X}) - g_k^L(\alpha_0^T \mathbf{X} - \tau_k^L)| \leq \frac{\epsilon}{8M_1} \quad \text{and} \quad \mathbb{E}|g_k^U(\alpha_0^T \mathbf{X} + \tau_k^U) - g_k^L(\alpha_0^T \mathbf{X})| \leq \frac{\epsilon}{8M_1}.$$

By picking $\tau = \min\{\tau_1^L, \dots, \tau_N^L, \tau_1^U, \dots, \tau_N^U\}/a$ (which implicitly depends on α_0), we claim that the class of functions

$$\tilde{g}_k^L(\mathbf{x}) = 2M_1(g_k^L(\alpha_0^T \mathbf{x} - \tau a) - 1/2)\mathbb{1}_{\{\mathbf{x} \in [-a, a]^d\}}, \quad \tilde{g}_k^U(\mathbf{x}) = 2M_1(g_k^U(\alpha_0^T \mathbf{x} + \tau a) - 1/2)\mathbb{1}_{\{\mathbf{x} \in [-a, a]^d\}}$$

for $k = 1, \dots, N_3$, form an ϵ -bracketing set in the $L_1(P_{\mathbf{X}})$ -norm for the set of functions

$$\begin{aligned} \mathring{\mathcal{F}}_{a, M_1}^{\alpha_0, \tau} = \left\{ \mathring{f} : \mathbb{R}^d \rightarrow \mathbb{R} \mid \mathring{f}(\mathbf{x}) = f(\alpha^T \mathbf{x})\mathbb{1}_{\{\mathbf{x} \in [-a, a]^d\}}, \text{ with } f : \mathbb{R} \rightarrow \mathbb{R} \text{ increasing,} \right. \\ \left. \sup_{x \in \mathbb{R}} |f(x)| \leq M_1 \text{ and } \|\alpha - \alpha_0\|_1 \leq \tau \right\}. \end{aligned}$$

To see this, we note that

$$\sup_{\|\alpha - \alpha_0\|_1 \leq \tau, \mathbf{x} \in [-a, a]^d} |\alpha^T \mathbf{x} - \alpha_0^T \mathbf{x}| \leq \tau a.$$

It follows by monotonicity that for $k = 1, \dots, N_3$,

$$\begin{aligned} \mathbb{E}|\tilde{g}_k^U(\mathbf{X}) - \tilde{g}_k^L(\mathbf{X})| &\leq 2M_1\mathbb{E}|g_k^U(\alpha_0^T \mathbf{X} + \tau a) - g_k^U(\alpha_0^T \mathbf{X})| + 2M_1\mathbb{E}|g_k^U(\alpha_0^T \mathbf{X}) - g_k^L(\alpha_0^T \mathbf{X})| \\ &\quad + 2M_1\mathbb{E}|g_k^L(\alpha_0^T \mathbf{X}) - g_k^L(\alpha_0^T \mathbf{X} - \tau a)| \leq \frac{\epsilon}{4} + \frac{\epsilon}{2} + \frac{\epsilon}{4} = \epsilon. \end{aligned}$$

Therefore, $\{\tilde{g}_k^L, \tilde{g}_k^U\}_{k=1}^{N_3}$ is indeed an ϵ -bracketing set.

Now for every $\alpha_0 \in \mathbb{R}^d$ with $\|\alpha_0\|_1 = 1$, we can pick $\tau(\alpha_0) > 0$ such that a finite ϵ -bracketing set can be found for $\mathring{\mathcal{F}}_{a, M_1}^{\alpha_0, \tau(\alpha_0)}$. Since $\{\alpha_0 \in \mathbb{R}^d : \|\alpha_0\|_1 = 1\}$ is compact, we can pick $\alpha_0^1, \dots, \alpha_0^{N^*}$ such that

$$\{\alpha_0 \in \mathbb{R}^d : \|\alpha_0\|_1 = 1\} \subseteq \bigcup_{k=1, \dots, N^*} \{\alpha \in \mathbb{R}^d : \|\alpha - \alpha_0^k\|_1 \leq \tau(\alpha_0^k)\}.$$

Consequently, for every $\epsilon > 0$, a finite ϵ -bracketing set can be found for $(\mathring{\mathcal{F}}_{a, M_1, M_2}^{\mathbf{L}_d})_j$. Finally, we complete the proof by applying Theorem 2.4.1 of van der Vaart and Wellner (1996). \square

Average running time per dataset (in seconds): Gaussian

Problem 1

Method	$n = 200$	$n = 500$	$n = 1000$	$n = 2000$	$n = 5000$
SCMLE	0.13	0.34	0.90	1.86	7.35
SCAM	0.91	1.72	4.17	7.43	18.59
GAMIS	0.11	0.20	0.46	1.46	3.93
MARS	0.01	0.01	0.02	0.05	0.12
Tree	0.01	0.01	0.02	0.03	0.08
CAP	0.61	1.75	2.47	3.86	8.60
MCR	30.17	411.80	-	-	-

Problem 2

Method	$n = 200$	$n = 500$	$n = 1000$	$n = 2000$	$n = 5000$
SCMLE	0.07	0.18	0.37	0.88	3.03
SCAM	2.85	3.27	6.26	12.22	29.78
GAMIS	0.11	0.20	0.44	1.39	3.92
MARS	0.01	0.01	0.02	0.04	0.09
Tree	0.01	0.01	0.02	0.03	0.07
CAP	0.11	0.32	0.55	0.97	1.93
MCR	33.31	427.98	-	-	-

Problem 3

Method	$n = 200$	$n = 500$	$n = 1000$	$n = 2000$	$n = 5000$
SCMLE	0.35	0.95	2.37	5.41	20.21
SCAM	23.08	25.77	38.60	70.67	143.91
GAMIS	0.45	0.60	1.10	3.19	8.09
MARS	0.01	0.02	0.04	0.08	0.22
Tree	0.01	0.02	0.03	0.05	0.12
CAP	0.10	0.37	0.99	1.83	4.20
MCR	26.61	303.40	-	-	-

Table 13: Average running time (in seconds) of SCMLE, SCAM, GAMIS, MARS, Tree, CAP and MCR on problems 1, 2, 3 with sample sizes $n = 200, 500, 1000, 2000, 5000$ in the Gaussian setting.

Average running time per dataset (in seconds): Poisson and Binomial

Problem 1

Model	Method	$n = 200$	$n = 500$	$n = 1000$	$n = 2000$	$n = 5000$
Poisson	SCMLE	0.33	0.78	1.76	3.98	13.08
	SCAM	1.24	2.40	4.92	9.99	30.54
	GAMIS	0.25	0.50	1.00	2.43	7.08
Binomial	SCMLE	0.24	0.53	1.23	3.22	9.51
	SCAM	0.80	1.09	1.92	5.24	9.06
	GAMIS	0.25	0.47	0.93	2.49	6.66

Problem 2

Model	Method	$n = 200$	$n = 500$	$n = 1000$	$n = 2000$	$n = 5000$
Poisson	SCMLE	0.20	0.41	0.84	1.80	5.10
	SCAM	1.97	2.67	5.17	11.34	25.35
	GAMIS	0.24	0.42	0.94	2.43	6.62
Binomial	SCMLE	0.16	0.35	0.72	1.49	4.63
	SCAM	1.82	3.06	6.38	9.60	25.87
	GAMIS	0.24	0.47	0.94	2.34	6.59

Problem 3

Model	Method	$n = 200$	$n = 500$	$n = 1000$	$n = 2000$	$n = 5000$
Poisson	SCMLE	0.90	2.29	5.59	12.68	42.58
	SCAM	8.85	16.93	22.77	39.69	77.08
	GAMIS	0.91	1.62	2.99	7.02	19.01
Binomial	SCMLE	0.46	1.10	2.50	5.37	18.54
	SCAM	5.80	6.29	8.73	14.10	30.07
	GAMIS	1.18	1.53	2.83	6.93	16.41

Table 14: Average running time (in seconds) of SCMLE, SCAM and GAMIS on problems 1, 2, 3 with sample sizes $n = 200, 500, 1000, 2000, 5000$ in the Poisson and Binomial settings.

Average running time per dataset (in seconds):

Additive Index Models

Problem 4

Method	$n = 200$	$n = 500$	$n = 1000$	$n = 2000$	$n = 5000$
SCAIE	4.36	6.61	12.20	23.50	69.52
SSI	26.10	112.44	411.16	1855.37	-
PPR	0.01	0.01	0.01	0.02	0.05
MARS	0.01	0.03	0.05	0.10	0.25
Tree	0.01	0.01	0.01	0.03	0.03
CAP	0.48	1.24	1.90	3.02	6.69
MCR	38.21	496.54	-	-	-

Problem 5

Method	$n = 200$	$n = 500$	$n = 1000$	$n = 2000$	$n = 5000$
SCAIE	3.78	8.76	20.32	62.68	203.20
PPR	0.01	0.02	0.03	0.05	0.12
MARS	0.01	0.01	0.02	0.03	0.04
Tree	0.01	0.01	0.01	0.02	0.03

Table 15: Average running times (in seconds) of different methods for the shape-constrained additive index models (Problems 4 and 5).